일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PLEN-1**
발표분야: 기조강연
발표종류: 특별강연, 발표일시: 목 11:00, 좌장: 이남수

Compensated Heat, Uncompensated Heat, Generalized Thermodynamics, and Generalized Hydrodynamics

Byung Chan Eu

McGill University, Canada

The science of thermodynamics was initiated 160 years ago, and its basic principles underlie our understanding of how all macroscopic natural phenomena work, but the implementation of the basic principles is an as-yet-unfinished business and still evolving, contrary to the popular perception of the status of thermodynamics as a finished subject. Here I would like to discuss a step toward an improved formulation of thermodynamics over the classical formulation of Clausius and Gibbs, J. W., by removing an important restriction of the Clausius formulation. First, the notions of compensated and uncompensated heats will be discussed. Therewith the Clausius inequality will be cast into an equation for the mathematical representation of the second law of thermodynamics. It will be shown the Clausius inequality can be recast into an equation (in fact, a differential form), if the uncompensated and compensated heats are recognized as physically different and independent quantities. This recognition naturally gives rise to a new notion, calortropy (heat evolution), that replaces the Clausius entropy for reversible processes on which equilibrium thermodynamics for reversible (equilibrium) processes is founded. This notion of calortropy enables us to incorporate a generalized form of classical hydrodynamics---namely, generalized hydrodynamics---into a thermodynamically consistent macroscopic theory of irreversible processes occurring in material systems far removed from equilibrium. This theory makes it possible to study irreversible phenomena at arbitrary degree of removal from equilibrium in a thermodynamically consistent manner. Some examples of applications of the theory will be shown for shock wave structures in regimes beyond the transient regime, for example, in high Mach number flow in gas dynamics, and rheology of highly sheared fluids, simple or complex, or chemical pattern formation and wave propagation. * Work supported in part by the Discovery grants from the Natural Sciences and Engineering Research Council of Canada.

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발표분야: 기조강연
발표종류: 특별강연, 발표일시: 목 11:45, 좌장: 김기문

Carbon nanotubes in materials science and nanomedicine

Maurizio Prato

University of Trieste, Italy

Among the wide variety of novel nanometer scale structures available, single-wall carbon nanotubes (SWNT) and multi-wall carbon nanotubes (MWNT) stand as unique materials for fundamental research and potential applications. However, manipulation and processing of NTs has been difficult because of their intractability and insolubility in most common solvents. Considerable effort has therefore been devoted to the chemical modification of NTs, which might pave the way to many useful applications. Our group has been involved in the organic functionalization of various types of nanocarbons, including carbon nanotubes, nanohorns, fullerenes, graphene and nanoonions. Organic functionalization allows novel applications in such diverse fields as materials science and nanomedicine. For instance, functionalized carbon nanotubes enhance neuronal communication or can serve as carriers for innovative drug delivery systems. On the other hand, carbon nanotubes are ideal supports for catalysis useful in water splitting devices.During this talk, we will report on the most recent advances in our group, which have led to several interesting applications in many fields.

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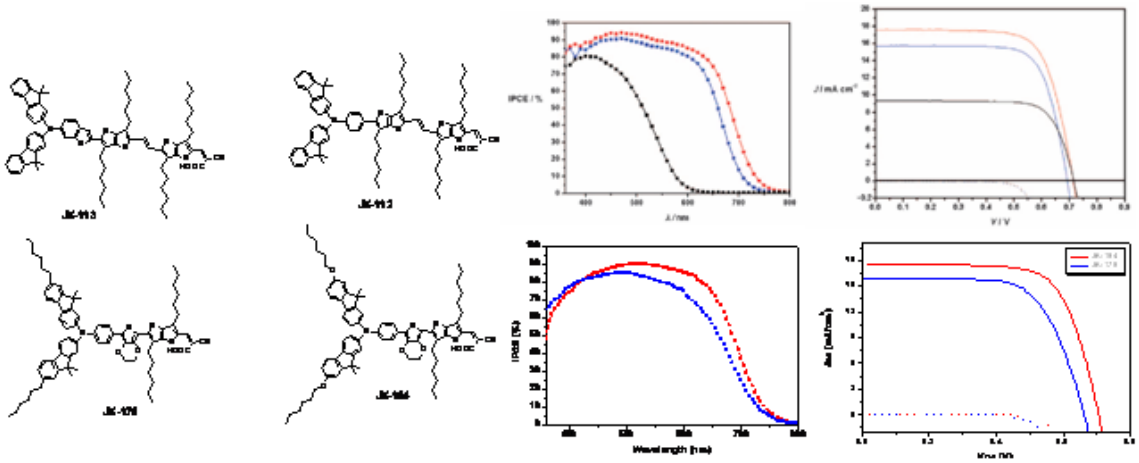
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 목 13:30, 좌장: 김진흥

Molecular Engineering of Highly Efficient Dye-Sensitized Solar Cells

고재중, 최현봉, 김철우, 백상현, 조나라, 임기민, 도광석, 최혜주, 소슬기, 김경준, 최홍식, 정반석, 유태정, 송주만

고려대 소재화학과

The current global warming and depletion of fossil fuels have created an urgent need to develop new renewable energy sources. Dye sensitized solar cells (DSSCs) represents one of the most promising candidates due to their low cost and high efficiency. In these cells, the sensitizer is one of the key components for DSSCs. Over the last 19 years, ruthenium sensitizers have achieved remarkable efficiencies over 11% under standard air mass 1.5 sunlight. However, there are still many problems to be addressed in terms of the rarity of precious ruthenium metal and their synthetic high cost. In this regard, organic sensitizers might be considered as an alternative to ruthenium sensitizers. 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, which consist of a dimethylfluorenylamino-appended thienothiophene–vinylene–thienothiophene unit with aliphatic chains that maintain the planar geometry of the conjugated linker. This not only increases the extinction coefficient of the sensitizer by extending the p-conjugation of the bridging linker, but also augments its hydrophobicity, increasing the stability under long-term light soaking and thermal stress. Also, for obtaining high photovoltaic performance from organic DSSCs is based on the structural modification of the dye because small structural changes of dyes result in significant changes for the interfacial recombination and absorption behavior of the dyes on TiO_2 surfaces. A successful molecular engineering was achieved by incorporating long alkyl groups into the spacer group and triphenylamine derivatives which not only increased the photoconversion efficiency but also minimized charge recombination. As part of our efforts to investigate the structural modification of spacer group that can suppress aggregation as well as broaden UV spectrum, we adapted a binary π–conjugated spacer.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **AWARD-2**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 목 17:00, 좌장: 이남수

Organization of Nano and Micro Building Blocks into Functional Materials

윤경병

서강대 화학과

Atoms and small molecules are well-known building blocks in chemistry and materials science. Nanoparticles and microparticles have begun receiving great attention as a new class of building blocks for the production of innovative materials. It is therefore necessary to start developing the methods of organizing them into larger organized products and to explore practical applications of the organized products. With this background in mind we have developed various methods of organizing silica nanoparticles and zeolite microparticles into closely packed and uniformly aligned mono and multilayers on various substrates. The produced zeolite mono and multilayers have served as supramolecularly organized light harvesting systems and as excellent precursors for the preparation of continuous zeolite films with uniform nanopore or nanochannel orientations that are useful for molecular sieving membranes and nonlinear optical films. The highly organized mono and multilayers of silica nano particles will be widely used as photonic materials. Various interesting features of the assembly of silica nanoparticles and zeolite microcrystal and the novel applications of organized products for advanced materials will be presented.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 원종옥

문화재보존과 화학 - 소개

도춘호

순천대 나노신소재응용공학부

문화재에 대한 관심과 문화재 보존에 대한 관심이 문화의 발전과 함께 점점 커지고 있다. 문화재의 변질과 손상은 물리적인 변화 이외에 화학적 변화가 주된 것이다. 문화재를 구성하는 재료의 분석과 검사, 보존 방법, 처리 및 복원, 그리고 보존과 문화재의 진위 확인 등은 모두 화학의 지식과 기술에 기반을 두고 있고 따라서 화학적 지식과 기술 그리고 화학자의 참여와 역할이 중요하다. 이 심포지엄을 통해서 우리나라 및 외국의 문화재 보존에 응용되는 화학 지식과 기술과 현황에 대해서 논의하고자 한다. 문화재 보존에 관한 학회가 있기는 하지만, 화학자들의 참여가 더욱 요구되는 마당에 대한화학회 내에 관련 분과회를 조직하여서 문화재 보존에 대해 화학자들이 문화재 보존에 참여하는 계기를 마련하고자 한다.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 원종옥

Cultural heritage know means to protect

Luigi Campanella

Italian Chemical Society

The protection of cultural heritage is not just an action but rather a process through different phases.knowledge,restoration,consolidation.The knowledge is referred to the basic material and its transformations due to the ageing and the impact from the environment,to the techmology of building,to provenance,to age.Restoration changed its meaning during the centuries passing from a rebuilding position to one more respecting the original manufact,Any way it applies different technologies and methods coniugating the stop to the damage and the elimination of any added compound due to the action of time or environment.Finally it is needed to avoid that the damage is rapidly repeated and this requires correction of materials and/or environment.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 원종옥

A Novel Method to Measure the Penetration Depth of Silicate Consolidants for Stone Conservation

강용수

한양대 화학공학과

A novel method to measure penetration depth of silicate consolidants through weathered stones is investigated. Although silicate consolidants is commonly used to conserve stone heritage. The stadard method to measure the penetration depth of the consolidants is not established yet. The penetration depth should be estimated precisely because the surface transport distance in a cubic stone sample has been unintentionally regarded as the penetration depth. However, we previously revealed that the penetration depth is totally different from the surface transport distanse. Therefore, a new dye was synthesized and utilized to measure the penetration depth. Even though the real penetration depth can be measured through the cross-section of the stone sample, it is not easy to notice the real penetration depth after completion of hardening process. Dye Red 336 (Hyundae Chemical Co.) has been commonly used to measure the penetration depth of consolidants with its clear deep red color. However, it has poor compatibility with silicate consolidants, showing different transport distance of Silres OH100 from Wacker Co. through surface and cross-section. For this reason, a novel dye molecule was synthesized, which is miscible with silicate consolidants. Therefore, it can be assumed that the traveling distance of the dye is the same as that of the consolidant. Then, the silicate consolidants with the new colorful dye molecule can be visible after their consolidation, and the penetration depth can be preciesly measured through the cross section of the sample because the transport distance of the consolidant and dye will be the same.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 원종옥

칠백의총 중봉조헌선생일군순의비의 과학적 보존처리와 복원

김사덕

국립문화재연구소 문화재보존과학센터

석조문화재의 보존처리에 사용되는 재료나 처리방법은 현대과학의 발달과 함께 급속히 변화하고 있다. 불과 10 년 전에 사용되었던 재료나 방법이 현재에는 새로운 재료와 방법으로 대체되기도 하며 이전에 복원한 원형이 새로운 자료의 발굴, 연구를 통해 다시 수정되기도 한다. 그러나 과거의 보수와 정비의 대부분은 철저한 고증 없이 문화재에 발생한 시급한 문제에만 국한하여 보존처리를 진행하여 왔다. 중봉조헌선생일군순의비도 1971 년에 복원이 이루어졌으나 잘못된 복원에 따른 보존상에 많은 문제를 가지고 있었다. 1603 년에 건립된 칠백의총 중봉조헌선생일군순의비(이하 순의비)는 임진왜란 당시 왜군에 맞서 순절한 칠백의사를 기리는 석비이다. 이 비는 일제시대(1940 년)에 폭파되는 수난을 겪은 후 1971 년에 복원되었으나 잘못된 복원에 따른 형태왜곡, 구조적 불안정, 복원 재료의 표면 이질감 등의 문제가 나타난 상태였다. 특히 비신의 일부 편과 이수는 접합하지 않은 채로 비의 주변에 보관되어 있었으며 유실되었던 비좌는 원형과 상관없이 비신을 세우기 위한 단순한 형태로 복원되었다. 이에 국립문화재연구소에서는 비를 해체 및 이관하여 과학적 보존처리와 복원작업을 시행하였다. 이 연구에서는 과학적인 분석을 기초로 처리방안을 마련하고 이를 토대로 진행된 순의비의 보존처리 및 복원 과정을 보고하고자 한다. 먼저 2007 년 8 월에 이수 편을 국립문화재연구소로 이송하였고, 2008 년 10 월에 비신의 해체와 함께 순의비의 복원을 위한 기초조사와 보존처리를 시작하였다. 기초조사에서는 순의비의 재질분석과 산지추정 연구를 수행하였으며 이를 근거로 정밀보존처리와 함께 결손부의 복원을 실시하였다.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 강용수

미술과 화학의 융합

전창림

홍익대 화학시스템공학과

미술은 시각예술이다. 시각적으로 표현하기 위해서 재료가 필요하다. 그 재료는 모두 화학적으로 제조되고 사용되고 보존되고 변화한다. 가치가 있는 미술 작품이라면 온갖 화학적 과정을 거쳐 후대에 문화재로 남겨질 것이다. 재료의 화학적 성질을 잘 알지 못하면 작가의 의도대로 재료를 사용하기 어렵고, 작가의 건강을 해칠 수도 있으며, 시간이 지나면서 의도하지 않았던 형태로 변화되거나 손상될 수도 있다. 미술과 과학의 접점에 있는 학문은 문화재보존과학이나 색채과학 정도일 것이다. 작가가 제작하고 오랜 시간이 지난 미술품을 오래도록 손상없이 잘 보존하는 것뿐 아니라, 이미 손상된 미술품을 분석하고 연구하여 원래의 색으로 되돌려 놓는 보수도 중요하다. 서양의 미술관들은 옛 대가들의 작품들을 때만 벗겨 내는 것이 아니라 현대의 불변성 안료로 새로 채색하여 원래 작가의 미술을 복원하는 일을 중요시한다. 컬러리스트라는 전문가를 배출하고 있는 색채과학은 일반적으로 광학, 색채응용만 포함하고 있다. 광학은 색채 스펙트럼이 어떻게 나타나고 측정될 수 있는지를 기술한다. 또한 색채응용은 색채의 심리적인 성질을 정리하여 건축, 디스플레이, 디자인 등에의 응용을 위한 색채의 조화, 대비, 효과 등을 연구한다. 그러나 정작 그 색채를 구현하는 수단인 재료 화학적인 면은 다루어지지 않았다. 화학과 미술의 복합학제적인 학자가 부족했던 것이 아니었나 생각된다.

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발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 강용수

석조문화재 손상도 평가를 위한 비파괴 초정밀 안전진단 및 모니터링 기술

이찬희, *서만철, 조영훈

*공주대 문화재보존과학과 *공주대 지질환경과학과*

석조문화재의 손상을 미연에 방지하기 위해서는 체계적인 보존시스템 정립과 비파괴 초정밀 안전진단 및 모니터링 기술이 필요하다. 이러한 비파괴 안전진단 및 모니터링 기술에는 표면 손상도를 정량적으로 평가하는 훼손지도, 암석의 강도를 비파괴 기법으로 측정하는 초음파 기술, 구조적 변위 분석에 활용되는 3 차원 영상분석, 거동 모니터링에 이용되는 틸트미터 계측 등이 있다. 훼손지도는 석조문화재의 물리적, 화학적, 생물학적 및 인위적 손상요인을 각각 기호화하고 모든 부재에 대한 풍화 및 종합 훼손상태를 수치로 나타내어 정량적으로 평가하는 방법이다. 초음파 측정은 석조문화재 구성석재에 대한 미세균열의 발달 정도 및 광물의 풍화정도에 따라 초음파속도가 달라지는 원리를 이용하는 방법이다. 이를 통해 구성석재의 풍화정도를 추정할 수 있고, 궁극적으로 암석의 강도도 산출할 수 있다. 3 차원 영상분석은 레이저 스캐닝으로 3 차원 형상 자료를 획득하여 석조문화재의 디지털복원을 완성하는 방법이다. 특히 이 디지털복원 결과는 후처리를 통해 변위분석을 수행할 수 있어 석조문화재의 구조적 안정성도 평가할 수 있다. 틸트미터 모니터링 기술은 실시간으로 석조문화재의 거동을 분석하여 구조적 변위 및 붕괴에 대한 사전예방을 가능하게 한다. 이러한 비파괴 안전진단 및 모니터링을 활성화하기 위해서는 석조문화재에 적합한 다양한 기법을 개발하고, 각 기법들의 신뢰도를 향상 시킬 수 있는 방안이 지속적으로 연구되어야 할 것이다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES1-7**
발표분야: 문화재 보존과 화학
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 강용수

물반응 실험을 통한 석조문화재 보수 무기질바인더의 안정성 연구

Study on the stability of inorganic binder as repair material of stone monuments through the reaction with water

도진영, 김대식

경주대 문화재보존학과

Mg, K, Si 와 소량의 Al 을 주 화학성분으로 하는 무기질바인더를 다양한 산성도의 물과 반응시켜 그 변화를 연구함으로서 석조문화재 보수물질로서의 적용가능성을 살펴보았다. 순수무기질바인더 1 종(A)과 이를 바탕으로 첨가제가 포함된 무기질바인더 3 종(B, C, D), 총 4 종을 대상으로 무기질바인더에 대한 시험을 실시하였으며, 화강암시편에 무기질바인더를 적용하여 암석에 미치는 영향을 관찰하였다. 국내 강우의 산성도와 함유이온을 토대로 pH 4.0 과 pH 5.6 의 강우를 제조하여 무기질바인더에 적용 후 무기질바인더의 변화와 그에 따른 암석의 변화양상을 관찰하였다. 이와 더불어 pH 8.0 강우와, 이온이 함유되지 않은 pH 7.0 강우도 적용하여 산성비에 대한 비교 자료로서 확보하였다. 무기질바인더는 물에 침수시키고, 암석시료에 부착한 무기질바인더에는 주사기를 이용하여 총 40 일간 물을 적용하였다. 무게측정결과, 물의 산성도에 따른 무게변화 차이는 뚜렷하지 않았고, 무기질바인더 A, D 가 B, C 에 비해 무게감소율이 2 배 이상 높았다. 일축압축강도 결과 역시 물의 산성도에 따른 차이는 무시할 정도였으나, 무기질바인더의 종류에 따라서는 차이가 크게 나타났다. 물과 반응전, 무기질바인더 A, D 의 강도는 B, C 에 비해 컸으나, 반응 후에느 A, D 의 강도감소율이 더 커졌다. 측정된 색상변화에서도 물의 산성도와는 관련이 적은 결과를 보였으나, 무기질바인더의 종류에 따라서는 큰 색상변화를 보였으며, 그 색상차는 A, D, C, B 순으로 나타났다. 물과 반응전 무기질바인더의 물흡수율은 1.05 ~ 11.95 wt.%의 높은 값을 보였으며, 물과 반응후에는 무기질바인더 D, A, B, C 의 순으로 큰 변화를 보였다. 물과의 반응에 의해 모든 무기질바인더에서 균열이 발생하였으며 무기질바인더와 암석 사이에서도 이격이 발생하였다. pH 4.0, 5.6, 7.0 및 8.0 의 인공강우가 모든

무기질바인더와 반응한 후 pH 9.0 이상의 알칼리성으로 변화하였다. 무기질바인더와 반응한 물에서 Na^{2+}, Mg^{2+}, K^{+}이 월등히 증가하여 무기질바인더로부터 용해되어 나왔음이 확인된다. 이러한 이온들은 $MgSO_4 \cdot 4H_2O$, $MgSO_4 \cdot 6H_2O$ 와 KNO_3 와 같은 용해도가 높은 염을 형성한다. 이번 연구에 대상이 된 4 가지 무기질바인더는 물과의 반응으로 수용성 이온성분의 과다한 검출, 균열을 발생시키는 결과를 보여 석조문화재 보수물질로 적용하기에 안정적이지 못한 것으로 판단된다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES1-8**

발표분야: 문화재 보존과 화학

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 강용수

나노소재를 함유한 에폭시 접착제 연구

원종옥

세종대 화학과

석조 문화재 보존을 위해 색안정성이 있는 에폭세계 접착제를 연구하였다. 에폭시 주제로 불포화결합을 수소화시켜 포화결합상태의 hydrogenated-bisphenol A (HBA)계 오폭시 수지로, 경화제로는 상온에서 경화가 가능한 아민계를 사용하였다. 낮은 기계적 강도를 향상시키기 위해 polyhedral oligomeric silsesquioxane 과 같은 나노소재를 함유한 복합 에폭시 접착제를 개발하였고, FT-IR 측정으로 경화도를, 인장강도, 압축강도, 굽힘강도 측정으로 기계적 특성을 확인하였다. 화강암에 적용하여 외부에 노출되어 있는 문화재 적용 가능성을 연구하였다.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES2-1**

발표분야: 녹색 화학과 녹색 성장

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 이규호

녹색 화학과 녹색 성장 - 소개, 녹색 성장과 화학자의 역할

도춘호

순천대 나노신소재응용공학부

녹색 화학이라는 용어는 꽤 오래전부터 사용되고 있고, 자원의 재활용, 에너지 절약, 효율의 극대화, 환경 친화, 지속적인 성장 등의 의미와 행동을 요구한다. 한편, "녹색 성장"은 저탄소, 에너지 절약, 지속가능성, 환경 친화적이라는 용어와 함께 우리나라의 새로운 산업과 사회 발전 방향과 동력으로 정의되고 추진되고 있다. 녹색 성장의 바탕에는 화학이 그 바탕을 이루고 화학의 지식과 기술이 활용되고 또 새로운 화학관련 지식과 기술의 발전을 필요로 한다. 대한화학회에서도 "녹색 화학 위원회"를 조직해서 화학자들이 녹색 화학과 녹색 성장의 기반을 살펴보고 적극적으로 참여할 수 있도록 준비하고 있다. 그리고 이번 심포지엄을 통해서 녹색 성장을 이해하고 녹색 화학을 통한 성장 방법과 방향을 토의하고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES2-2**
발표분야: 녹색 화학과 녹색 성장
발표종류: 심포지엄, 발표일시: 금 14:10, 좌장: 이규호

Present and Future of Advance Secondary Batteries in Korea

박정기

KAIST 화학공학과

Lithium ion batteries have been widely used in everyday life especially for mobile electronics, from cellular phones to lap top computers. For the last decade, there has been a very remarkable development in lithium ion battery technologies for the mobile applications. This rapid growth of battery technologies was possible owing to good combinational efforts between industries and government.Research and development on batteries for green cars are now under active progress in many countries. It is generally viewed, however, that the current technology for batteries of green car is still in an infant stage. We may have to go quite a long way to completely address all the problems on realization of the economic green cars. The renewable energy systems require also batteries with higher capacities, high performance, and low cost than current lithium ion batteries. For these, medium and large-sized lithium ion battery projects have been launched in the middle of the last decade. In this presentation, the past, present, and future of the lithium battery developments in Korea will be discussed. The roadmap for advanced battery technology development until 2015 in Korea is also introduced.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES2-3**

발표분야: 녹색 화학과 녹색 성장

발표종류: 심포지엄, 발표일시: 금 14:35, 좌장: 이규호

화학산업과 녹색화학기술

이규호

한국화학연구원 그린화학연구단

화학산업은 지난 반세기동안 우리나라를 대표하는 주력산업으로서 경제발전의 중추적인 역할을 담당하여 왔다. 그러나 에너지 위기와 지구온난화에 대한 대안과 삶의 질에 대한 강한 사회적 요구에 따라 지속적 성장을 의미하는 녹색성장과 이를 위한 녹색기술에 대한 중요성이 어느 때보다 커지고 있다. 이를 위해 화학산업은 기존의 석유화학산업의 에너지 저소비산업으로의 고도화, 바이오 화학산업 창출, 화학원천소재 개발을 통한 정밀화학 분야의 고부가가치화 등 을 통해 지구온난화 문제와 에너지 문제를 해결하고 국가산업과 경제를 재도약시키는 중요한 연결고리 역할을 해야 할 것이다. 화학은 많은 과학 분야의 기반이 되는 기초과학이자 화학기술은 주력기간산업의 융복합기술에 활용되는 핵심기반기술이다. 본 발표에서는 녹색성장을 위한 화학산업의 발전 방향과 이를 위한 녹색화학기술을 그동안 화학연구원에서 수행되고 있는 연구내용을 중심으로 소개하고 화학산업의 나갈 방향에 대하여 토론할 기회를 갖고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES2-4**
발표분야: 녹색 화학과 녹색 성장
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 이규호

정삼투 공정 연구 개발 현황

홍승관

고려대 건축사회환경공학부

지구온난화로 인한 기후변화는 전 세계적으로 수자원 고갈 및 수질저하 문제를 야기하여 해수담수화 및 물 재이용 등 대체 수자원 확보의 필요성이 부각되고 있다. 여러 수처리 기술 중 멤브레인 공정은 대체 수자원 확보에 가장 적합한 기술로 기대 받고 있다. 하지만 기존의 가압식막 공정(예, 역삼투막(RO)공정)은 분리를 위해 고압을 사용하기 때문에 많은 전력을 필요로 할뿐 아니라, 막 오염도 심하여 화학세정이나 전처리 공정이 요구되는 등의 경제적, 환경적 문제점을 안고 있다. 이에 최근 크게 주목받고 있는 정삼투(FO)공정은 농도차에 의해 자연적으로 발생하는 삼투압 에너지를 이용하기 때문에 에너지 및 회수율 문제를 동시에 해결할 수 있는 이상적인 수처리 기술로 평가되고 있다. 정삼투 기술 개발은 1970 년대부터 시작되었으나 이상적인 유도용질의 부재로 인하여 상용화의 진척이 미진했다. 2000 년대에 들어서 NH_3/CO_2 의 유도용질 및 분리기술 개발을 시작으로 FO/MBR, FO/RO 등 hybird 공정과 FO 단독 공정에 관한 연구가 활발히 이루어지고 있다. 그 결과 FO 공정은 현재 미래 담수 및 수처리 분리막 분야에서 3 대 신기술로 손꼽히며 최근 국내에서도 국가과제를 중심으로 기초 및 상용화 연구가 진행 중이다. 구체적으로 FO 공정의 조기 상용화를 위해, FO 공정에 최적화된 막 및 모듈, 유도용액 분리기술, FO 공정 설계 및 운영에 관한 연구를 체계적으로 수행하고 있다. 본 발표에서는 FO 공정 분야의 선도 연구자인 미 예일대 Elimelech 교수의 연구 및 고려대와의 공동연구 내용을 중심으로 최근 연구 동향을 살펴보았다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES2-5**
발표분야: 녹색 화학과 녹색 성장
발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 이규양

바이오매스 기반 바이오리파이너리 기술과 화학산업

장종산, 황동원, 황인택, 황진수

한국화학연구원 바이오리파이너리 연구센터

석유자원의 점차적인 고갈은 화학산업 뿐만 아니라 국가 기간산업 전체에 커다란 영향을 미치고 국가의 지속적인 발전에 장해 요인이 될 것으로 예상된다. 이에 따라 새로운 원료와 대체 에너지원 확보를 위해 식물자원을 이용하여 바이오연료 및 화학제품을 생산하는 바이오리파이너리 기술이 이산화탄소 온실기체 저감문제에 대응하는 지속성장 기술로서 기대를 모으고 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. 본 발표에서는 바이오리파이너리의 중요한 분야인 바이오매스 유래 화학적 전환기술의 국내외 기술개발 현황, 문제점 및 개발 방향 등을 소개하고 토론할 기회를 갖고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES2-6**
발표분야: 녹색 화학과 녹색 성장
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 이규양

Green chemical reactions; use of natural biocatalysts for biotechnological applications

장윤석

포항공과대 환경공학부

Laccases are multi-copper oxidases that catalyze single-electron oxidations of phenolic compounds with the concomitant reduction of oxygen to water. Applicability of laccases has been highlighted due to green nature and versatile biochemical features of the enzymes. We, here, review current advances in laccase-catalyzed oxidations of naturally occurring phenols particularly focusing on laccase-mediator system and organic synthesis, and discuss how both the application strategies can mimic in vivo biometabolism to make the application processes much greener and to extend applicability of the green reactions.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES2-7**

발표분야: 녹색 화학과 녹색 성장

발표종류: 심포지엄, 발표일시: 금 16:35, 좌장: 이규양

저탄소 녹색성장 추진정책 방향

우기종

대통령 직속 녹색성장위원회 기획단장

- 왜 지금 저탄소 녹색성장이 필요한가? ○ 기후·환경위기 + 에너지·자원위기 ○ 변화하는 미래 - 녹색성장의 열매는? ○ 녹색성장 추진 현황 및 성과 ○ 향후 추진방향 - 녹색성장과 녹색화학

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES3-1**
발표분야: 화학과 뉴스미디어의 역할
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 윤웅찬

화학과 뉴스미디어의 역할 - 소개, 일반인의 화학에 대한 이해와 화학자의 역할

도춘호

순천대 나노신소재응용공학부

화학은 우리 일상 생활과 직결되어있으므로 화학에 관한 지식과 기술 그리고 영향 등은 일반인들의 상식으로도 필요하다. 화학에 관련된 지식과 기술, 유용성, 필요성을 일반 시민들은 사건이나 사고와 뉴스 해설 등 뉴스 미디어를 통해서 화학 관련 정보를 얻는 경우가 많다. 따라서 화학에 관한 올바른 지식과 기술을 일반 시민들에게 널리 알리는 일은 중요한데, 대부분 정규적인 교육만 강조한다. 일반 시민들에게 직접적으로 알리는 방법을 간과하는 경우가 많고 또 적절한 방법을 찾지 못하고 있다. 이번 심포지엄을 통해서 화학자들은 시민들에게 화학에 관한 지식과 정보에 대해서 매개 역할을 하는 뉴스 미디어의 역할과 관점을 이해하고 협력 방안을 모색하고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES3-2**
발표분야: 화학과 뉴스미디어의 역할
발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 윤웅찬

과학 잡지에서 화학 기사의 내용과 범위

이충환

동아사이언스

식품첨가물은 불가피한 선택인가? 오염된 지구를 되살리는 첨병은? 돌돌 말린 디스플레이를 가능하게 하는 것은? 무병장수(無病長壽)를 실현하는 신약을 개발하려면? 사랑은 두뇌의 화학작용인가? 화학은 생활에 깊숙이 들어와 있지만 이를 제대로 이해하고 있는 경우는 많지 않다. 일반 시민은 화학 지식과 기술 자체는 물론 그 중요성과 필요성을 대부분 뉴스미디어를 통해 접한다. 뉴스미디어 가운데 잡지는 신문과 방송에 비해 공간적, 시간적 제약을 덜 받고 좀 더 심층적인 분석이 가능하다. 특히 과학잡지는 전문성과 시의성을 바탕으로 화학 관련 정보를 심도 있게 전달하고 있다. 국내 대표적 과학잡지인 '과학동아'에서 20 여 년간 게재한 기사를 분석해 화학 기사의 정의, 과학 기사 중 화학 기사의 비중, 화학 기사의 종류 등을 살펴본다. 과학동아에 실린 화학 기사는 크게 기초 분야, 응용 분야(생활 및 문화, 산업 및 첨단기술), 특집 및 기획, 인터뷰, 노벨상, 입시 및 진로 등으로 나눠 볼 수 있다. 아울러 화학 분야에서 뉴스미디어로서 과학잡지의 역할과 과학잡지를 통한 대중 커뮤니케이션 방안도 제시한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES3-3**
발표분야: 화학과 뉴스미디어의 역할
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 윤웅찬

을 중심으로 한 과학 윤리, 도덕, 그리고 과학사 이야기

김형근

사이언스 타임스

모든 사람, 그리고 모든 직업에는 윤리와 도덕이 뒤따른다. 과학과 과학자의 윤리 도덕을 운운하는 것은 편파적일 수도 있다. 다시 말해서 왜 하필이면 과학자냐? 그러나 과학자에 대해 엄준한 잣대를 요구하는 것은 과학과 기술이 너무나 대단하기 때문이다. 칠판 속에서의 화학과 물리방정식이 엄청난 결과를 불러오기 때문이다.과학자가 존경받는 사회는 과학자들이 만들어가야 한다고 생각한다. 아인슈타인은 단순히 상대성이론을 발견한 그러한 과학자에서 끝나지 않는다. 그는 독일의 군국주의와 히틀러의 통치에 맞서 싸운 지식인이다. 독일 군국주의 시대의 프리츠 하버를 살펴본다. 그야말로 화학의 천재인 그의 인생역정을 살펴보면서 '과학자란 무엇인가?'라는 생각을 해본다.그리고 비전공자인 과학저술가의 눈으로 바라본 과학, 그리고 과학교육의 중요성을 살펴보려고 한다. 특히 3 년 전 서울에서 열린 세계화학교육자대회에서 취재했던 경험과 느낌을 이야기했으면 한다.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES3-4**

발표분야: 화학과 뉴스미디어의 역할

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 윤웅찬

대한화학회의 새로운 임무

손동운

국제신문 과학문화연구소

학회는 연구자들의 모임이지만 사회적 역할 수행 필요. 특히 과학계에서 소홀히 하기 쉬운 역사성과 정체성, 청소년 교육, 외국인 유학생에 대한 배려 등이 필요하다. -외국인 유학생 배려 - 특히 아시아권 유학생에 동료애, 일체감 제공-청소년 및 신입생을 위한 화학과 진로교육: 고전적 분야에서 연료전지, 디 스플레이, 석유화학 에너지, 방호 페인트, 뉴메디신 등-롤모델 제시: 화학 각 분야 선구적 인물 제시-화학 용어 국산화: 중국, 일본 번역용어는 청소년, 일반인에게 벽, 우리나라 근대 과학역사 100 년 넘었으니 각 학회 차원 정리, 전달 필요 예) 지질학 안산암(andesite), 각섬석, 휘석 등-화학법칙 배경이야기 제공 : 배경 지식 알려주지 않고 공식만 제시 예) 미적분 공식만 있는 것과 뉴턴/라이프치히 논쟁 제공은 달라

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **PRES3-5**

발표분야: 화학과 뉴스미디어의 역할

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 윤웅찬

화학, 언론과 친해지기

김요셉

대덕넷

화학은 국가 과학기술 및 산업계에서 중요한 비중을 차지하고 있음에도 불구하고, 일반 대중은 화학에 대한 중요성을 제대로 인식하지 못하고 있으며 오히려 부정적 인식이 마음 한켠에 자리잡고 있는 양상이다.21 세기 화학 분야를 신성장동력으로 삼고 국가적인 집중 투자를 펼치기 위해서는 대중의 화학기술의 중요성 인식과 올바른 공감대 형성이 시급하다.화학의 중요성과 올바른 인식을 확산하는데 있어 무엇보다 미디어의 역할이 중요하며, 화학과 미디어 간의 합리적인 관계 형성이 필요한 시점이라 할 수 있다.특히 화학 보도 사례를 중심으로 화학과 미디어 간의 현황을 짚어보고, 미래의 화학 미디어 커뮤니티 방향성을 고민하고 도출해 보는 노력이 필요하다.'화학, 언론과 친해지기'라는 주제발표는 화학 분야의 주요 취재과정과 보도사례 중심으로 발표될 예정이며, 화학 연구계 및 산업계가 좀 더 미디어를 잘 이해하고 대응할 수 있는 방안을 모색할 예정이다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PRES3-6**
발표분야: 화학과 뉴스미디어의 역할
발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 윤웅찬

화학 산업과 방송뉴스의 친해지기

선우석

ubc 울산방송

방송 뉴스에서 화학 산업의 뉴스란 대개 사건사고가 중심을 이루고 있다. 울산 지역의 경우 대규모 화학기업들이 밀집해 있는데 이들 기업에서 사고가 발생했을 경우 SBS 등 중앙방송을 통해 전국 뉴스로 전해지는 경우가 많다. 이 때문에 방송을 통해 전해지는 화학 산업에 대한 국민적인 인식은 국민의 생명과 안위를 위협하는 위험한 산업이라는 인식이 뿌리 깊게 내리고 있다. 화학 산업을 지역 최대 주력산업으로 두고 있는 울산지역 방송계가 이 같은 점을 고려해 석유화학산업의 뉴스를 많이 전하려고 하지만 우선 방송계 구조적인 문제점도 있다. 기사를 다루는 주체인 기자와 이를 수용하는 시청자 모두가 화학 산업의 기사를 쉽게 이해할 수 없다는 것이다. 기사를 다루는 주체인 기자의 경우 화학업계의 기사화 자체가 다른 분야에 비해 어렵다. 울산방송의 경우 보도국에 기자가 13~14 명이 있지만 이공계 출신은 단 한명도 없다. 이 때문에 담당기자도 화학업계 기사를 다루기가 어렵고, 기사 비중을 낮추는 경향도 있고 심층취재도 어렵다. 시청자 입장에서도 화학 산업의 기사는 우선 어렵다. 방송기사는 기사보다는 그림 위주인데 상대적으로 다른 분야 기사에 비해 그림으로 보여줄 것이 적고 또 어렵다.방송뉴스에서 화학 산업 기사가 자주 등장하기 위해서는 화학업계 관계자들이 우선 방송기자들과의 대면 접촉을 늘려서 언론의 '계몽' 기능을 높여야 한다. 화학 산업도 미디어와의 접촉을 늘리고 이를 강화함으로써 일반 국민들과 시청자들이 편안하게 화학 산업 용어들과 기본개념을 받아들여서 화학산업에 대한 이해도를 높일 수 있도록 해야 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **POLY1-1**
발표분야: 고분자 화학 첨단연구
발표종류: 분과기념강연, 발표일시: 목 14:00, 좌장: 조창기

Reverse Thermogelling Biodegradable Polymers and Their Biomedical Applications to Drug Delivery and Tissue Engineering

정병문

이화여대 화학나노과학과

An aqueous system that undergoes a sol-to-gel transition as the temperature increases (reverse thermal gelation) has been suggested as one of the most promising implantable systems of pharmaceutical agents and cells/stem cells due to its simple fabrication and non-surgical implanting procedure. We reported a series of reverse thermal gelling polymer systems including polyesters, polycarbonates, polycyanoacrylates, polypeptides, etc which have been cited about 3,000 times by colleagues during last decade. A brief summary of the polymer systems developed by our group will be presented, focusing characteristics, mechanism, and biomedical applications. References1. Choi, YY, Jang, JH, Park, MH, Choi, BG, Chi, B, Jeong, B, J. Mater. Chem. 2010, 20, 3416-3421.2. Joo, MK, Park, MH, Choi, BG, Jeong, B, J. Mater. Chem. 2009, 19, 5891-5905. 3. Jeong, Y, Joo, MK, Bahk, KH, Choi, YY, Kim, HT, Kim, WK, Sohn, YS, Jeong, B, J. Controlled Rel. 2009, 137, 25-30. 4. Kim, JY, Park, MH, Joo, MK, Lee, SY, Jeong, B, Macromolecules 2009, 42, 3147-31515. Han, JO, Joo, MK., Jang, JH, Park, MH, Jeong, B, Macromolecules 2009, 42, 6710-6715.6. Oh, HJ, Joo, MK, Sohn, YS, Jeong, B, Macromolecules 2008, 41, 8204-8209.7. Jeong, Y, Joo, MK, Sohn, YS, Jeong, B, Advanced Materials 2007, 19, 3947-3950.8. Suh, JM, Bae, SJ, Jeong, B, Advanced Materials 2005, 17, 118-120

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발표코드: **POLY1-2**
발표분야: 고분자 화학 첨단연구
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 백종범

산소부화막, OLED, OTFT, Solar cell용 기능성 고분자의 합성

권순기

경상대 나노신소재공학부

In the Gas Separation Membrane, oxygen permeability characteristics of cardo polyimides exhibited 150 x 10-10 cm3(STP) cm/(s cm2 cmHg). In the polymer lighting emitting diodes, blue emitting copolymer of alkoxynaphthalene and alkylfluorene show pure blue emitting of color coordinate at (0.15, 0.10). In the organic photovoltaic cell, copolymer of donor showed power conversion efficiency of 4.15 %. In the organic thin film transistors, thiophene containing polymer show high hole mobility of 0.12 cm2/Vs, and side chain conjugation polythiophene derivatives show high mobility of 0.05cm2/Vs and good air stability.

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발표분야: 고분자 화학 첨단연구
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 백종범

Protein detection using aqueous/LC interfaces decorated with SGLCP-b-polyacrylic acid block copolymers

박수영

경북대 고분자공학과

The functionalized interface between 4-cyano-4´-pentylbiphenyl (5CB) and water in the TEM grid by decoration of a amphiphilic block copolymer which consists of side-group liquid crystalline polymer (SGLCP) block and poly(acrylic acid) (PAA) block was examined for protein detection. Lysozyme, bovine serum albumin (BSA), ´ -lactalabumin, and insulin was found to make complexes with the protonated PAA chains at pH=12, which was transduced to 5CB through SGLCP block by the homeotropic to planar orientational change (PH change) of the 5CB. Lysozyme was selected for a model protein for screening the effects of pH, areal density of the monolayer and salt concentration on the protein detection performance of the flow cell because its isoelectric point (PI) of 11 is in the homeotropic orientation region of the 5CB in the flow cell. The PH change was observed when lysozyme was injected into the flow cell regardless of the state of the net charge of the protein. However, the speed of the PH change was strongly dependent on the pH, salt concentration and areal density of the monolayer controlled by the surface pressure (SP) of the Langmuir-Blodgett film. The speed of the PH change became slower as pH of the water increased above the PI of lysozyme due to delay of the complexation through the electrostatic repulsion between protonated PAA chains and negatively net charged protein. The speed of protein adsorption decreased as the areal density of the block copolymer monolayer on the 5CB increased, and the PAA chains became even protein-resistant at SP of higher than 45 mN/m. The speed of the protein adsorption became slow as the salt concentration increased. Finally, the performance of the flow cell was tested with human albuminuria. The lower limit of the concentration of protein in albuminuria was as low as 2.3 ´ M at SP=30 mN/m and pH=12 with addition of 1 M NaCl. We demonstrated the sensitivity of our flow cell by measuring adsorption of proteins, and are exploring its

use as a biosensor by employing selective protein detection units such as antibody and aptamer in the PAA chains.

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장소: 대구엑스코

발표코드: **POLY1-4**

발표분야: 고분자 화학 첨단연구

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 백종범

분자조립 연성나노소재

김상욱

KAIST 신소재공학과

고분자, 액정, 생체분자들을 포함하는 연성소재들은 분자들간의 상호작용에 의해 스스로 분자조립현상을 일으키는 경우가 많다. 본 발표에서는 블록공중합체나 탄소나노튜브, 그래핀등의 분자조립현상을 이용하여 초미세 나노소재들을 만드는 다양한 기술들을 소개할 것이다. 이들 나노소재들은 디스플레이나 반도체 또는 에너지소자의 전극등 다양한 분야에 이용될 수 있다.

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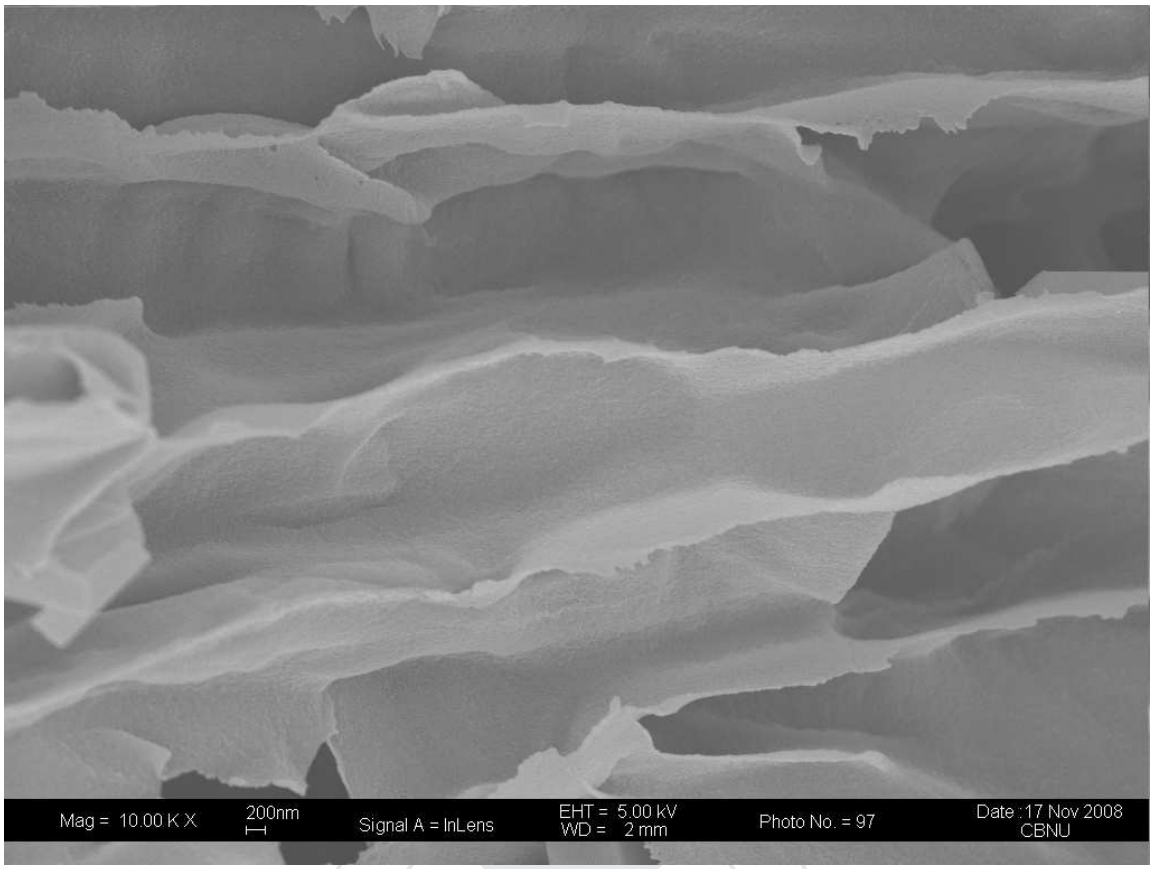
발표분야: 고분자 화학 첨단연구
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 김상욱

"Direct" Grafting of Linear Macromolecular 'Wedges' to the Edge of Pristine Graphite: A Precursor toward Exfoliation of Graphite into Two-Dimensional Graphene

백종범

울산과학기술대 에너지공학부

The edges of pristine graphite were covalently grafted with para-poly(ether-ketone) (pPEK) in a mildly acidic polyphosphoric acid (PPA)/phosphorous pentoxide (P¬2O5) medium. The resulting pPEK grafted graphite (pPEK-g-graphite) showed that the pristine graphite had been exfoliated into a few layers of graphene platelets (graphene-like sheets), which were uniformly dispersed into a pPEK matrix. As a result, the tensile properties of pPEK-g-graphite films were greatly improved compared to those of controlled pPEK films. The origins of these enhanced mechanical properties were deduced from scanning electron microscope (SEM) images of fracture surfaces. Upon tracing wide-angle x-ray scattering (WAXS) patterns of the film under strain, the graphene-like sheets were further exfoliated by an applied shear force, suggesting that a toughening mechanism for the pPEK-g-graphite film occurred. This approach envisions that the "direct" edge grafting of pristine graphite without pre-treatments such as corrosive oxidation and/or destructive sonication is a simple and efficient method to prepare graphene-based polymer composites with enhanced mechanical properties.



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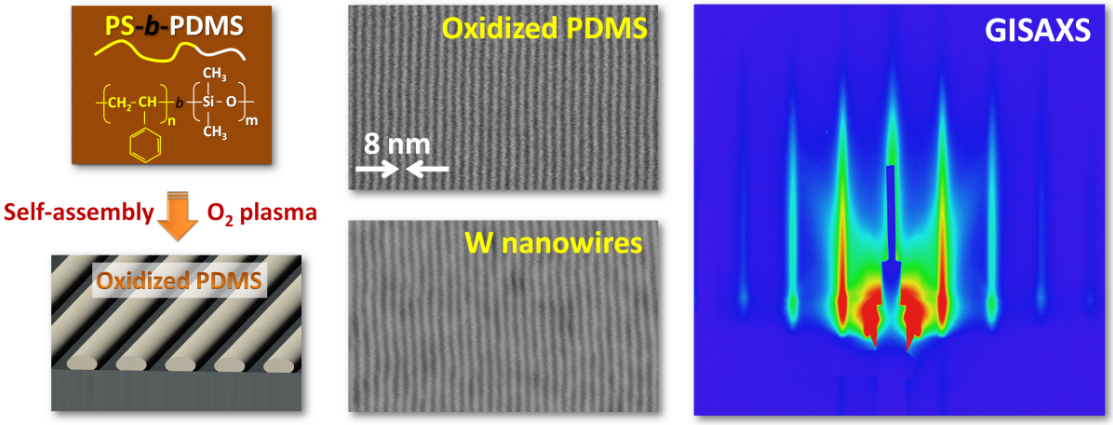
발표분야: 고분자 화학 첨단연구
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 김상욱

Self-assembled processing of siloxane block copolymers for nanolithography

정연식

KAIST 신소재공학과

Directed self-assembly of block copolymer (BCP) have been widely studied for applications in sub-20 nm nanolithography since BCP self-assembly is scalable and low cost, and is well-matched for conventional semiconductor manufacturing processes. However, the two critical issues are how to obtain reliable long-range ordering of features with minimum defect densities and how to successfully transfer the patterns into other functional materials. We can fabricate exceptionally well-ordered and robust 8 - 20 nm scale patterns from poly(styrene-b-dimethylsiloxane) (PS-PDMS) BCPs, which have a very large interaction parameter between the blocks compared to other commonly used BCPs. These can be used as an etch mask or an easily removable template for patterning functional materials. The self-assembly of a thin film of spherical or cylindrical morphology block copolymers can also be templated using an array of topographical elements. The orientation and periodicity of BCP patterns can be controlled by the commensurability between the block copolymer period and the template period. Procedures to transfer the generated patterns into various kinds of functional materials such as conducting polymers, graphene, organic photovoltaic materials, and metals are described as well.



대한화학회
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발표분야: 나노임프린팅 기술과 기능성 소재
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 도이미

TFT-LCD 적용 임프린팅 기능성 소재

김진욱, 채기성, 황용기, 정인재

엘지디스플레이 재료1팀

The column spacer and overcoat layer of the color filter substrate for liquid crystal displays formed at once by capillary force lithography was studied using UV-replica mold and UV curable liquid resin. The low viscosity and rapid curing speed of the liquid resin make it possible to pattern successfully in the industry application. We can estimate the coating thickness in order to achieve desired overcoat thickness according to mass balance. The formed overcoat layer and column spacer exhibited both satisfied transmittance and recovery ratio for liquid crystal display as commercial these for photo-lithography method. Finally, we demonstrated the panel using this technique and material. This work can provide a possibility for simply and low-cost process to form a functional layer in display.

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발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 도이미

Fabrication of an All-Layer-Printed TFT-LCD Device via Large-Area UV Imprinting Lithography

이승준

SAMSUNG ELECTRONICS LCD R&D Center

Nanoimprint lithography (NIL) by ultraviolet (UV) is a technique in which unconventional lithographic patterns are formed on a substrate by curing a suitable liquid resist in contact with a transparent patterned mold, then releasing the freshly patterned material. Here, we introduce various solutions to achieve the sufficient overlay accuracy and technical challenges for resist patterning by UV-imprinting. Also, resist patterning of all layers in TFT and BM layer in CF were carried out using UV-imprinting Lithography to make a 12.1 inch TFT-LCD panel at the resolution of 1280 x 800 lines (125 ppi).

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발표코드: **POLY2-3**

발표분야: 나노임프린팅 기술과 기능성 소재

발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 도이미

나노임프린트 리소그래피 시스템 기술

이재종

한국기계연구원

나노제품을 생산할 수 있는 나노기계는 반도체장비를 포함하여 최근에 세계적으로 중요한 기술로 인식되고 있는 나노임프린트 기술(NIL), 전자빔리소그래피(EBML), 극자외선 리소그래피(EUVL), 주사식프로브현미경(SPM) 등이 있다. 특히, 나노임프린트 기술은 나노형상을 가지고 있는 형틀(몰드)을 반복적으로 사용하여 나노제품을 대량으로 생산할 수 있는 기술이다. 최근에는 나노임프린트 기술을 이용하여 반도체 플래쉬메모리, 나노형상을 이용한 바이오/가스센서, 광통신소자, 단위면적당 1Terabit/in2 이상의 차세대 하드디스크드라이브를 제작할 수 있는 나노기계기술과 공정기술이 개발됨에 따라 다양한 나노제품을 생산할 수 있을 것으로 예상된다. 본 세미나에서는 나노임프린트 장비기술과 장비응용기술에 대해서 소개하고자 한다.

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Silicate Replica Molds for Nanoimprint Lithography

김동표

충남대 공업화학과

Silicate molds were fabricated from two types of inorganic-organic hybrid resins for UV- and thermal-nanoimprint lithography. SiO2-TiO2-PEG resins were used to replicate the features down to 80 nm with high fidelity through both nanoimprint lithography techniques. And the alternative silicate mold with easy releasing properties was fabricated by phase conversion hydrolysis of the cured polyvinylsilazane replica and used to fabricate 30~50 nm patterns through UV- and thermal nanoimprint lithography.

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발표분야: 나노임프린팅 기술과 기능성 소재
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 이승준

발광다이오드 소자의 광추출 효율 향상을 위한 기능성 물질의 직접 나노 패터닝 기술 연구

이헌

고려대 신소재공학과

최근 LED 소자의 다양한 장점들이 부각되면서 LCD back-light, 휴대용 전자기기, 조명기구 등 다양한 응용분야로 적용되고 있다. 하지만 보다 다양한 분야로 LED 소자가 적용되기 위해서는 기존의 LED 소자 보다 향상된 발광 효율이 필요하다. LED 소자의 발광 효율은 internal quantum efficiency 와 light extraction efficiency 에 의해 결정되는데 현재 GaN 의 MOCVD 기술의 발전에 의해 internal quantum efficiency 는 80~90%까지 향상되었으나 아직까지 light extraction efficiency 는 그에 미치지 못하고 있는 실정이다. LED 소자의 light extraction efficiency 를 향상시키기 위해 다양한 시도들이 진행되고 있는 가운데 LED 소자의 표면에 2 차원 광결정 구조를 형성하게 되면 LED 소자의 light extraction efficiency 가 비약적으로 향상된다는 다수의 연구 결과가 발표되고 있다. 하지만 기존의 나노 패터닝 기술을 이용하여 광결정 구조를 제작할 시에 필수적으로 필요한 건식 식각 공정에 의해 LED 소자의 표면에 형성되어 있는 TCO 층 혹은 p-GaN 층의 전기적 특성이 열화되는 문제가 발생되고 있다. 이러한 전기적 특성의 열화를 방지하면서 LED 소자의 light extraction efficiency 를 향상시키기 위해서는 높은 굴절율을 갖는 기능성 물질의 직접 나노 패터닝 공정을 통해 광결정 구조를 제작하는 기술에 대한 연구가 필요하다. 나노 임프린트 리소그래피 기술은 몰드와 임프린팅 레지스트와 접촉을 통해 몰드 표면에 형성되어 있는 나노 패턴을 임프린팅 레지스트층으로 전사하는 기술이다. 따라서 이러한 나노 임프린트 리소그래피 기술의 특성을 이용하게 되면 기능성 물질의 직접 나노 패터닝이 가능하다. 본 연구에서는 sol 용액과 nanoparticle 용액을 임프린팅 레지스트로 이용하여 나노 임프린트 리소그래피 공정을 진행함으로써 기능성 물질의 나노 패턴을 직접 형성하는 기술에 대한

연구를 진행하였고 이를 LED 소자로 적용하여 전기적 성질의 저하를 방지하면서 light extraction efficiency 를 향상시키는 기술에 대한 연구를 진행하였다.

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발표분야: 나노임프린팅 기술과 기능성 소재
발표종류: 심포지엄, 발표일시: 금 16:40, 좌장: 이승준

Photo-induced hybrid nanopatterning of titanium dioxide via direct imprint lithography

정준호

한국기계연구원 나노융합기계연구본부

A novel ultraviolet (UV)-assisted imprinting procedure that employs photosensitive titanium(IV) di-n-butoxide bis(2-ethylhexanoate) is presented for the fabrication ofwell-ordered titaniumdioxide (TiO2) nanostructures at room temperature. The main novelty of this technique is the use of the photosensitive titanium organic compound, rather than a commonly used UV-curable resin, for direct UV-assisted nanoimprint lithography.Fourier transform infrared andX-ray photoelectron spectroscopy studies suggest that exposure to UV light resulted in the gradual removal of organic groups from films prepared from titanium(IV) di-n-butoxide bis(2-ethylhexanoate) photochemically and successively converted the films to TiO2 at roomtemperature. This approach allows direct fabrication ofTiO2 nanopatternswith lines down to 35 nm in width, hole arrays of 265 nm in diameter, and three-dimensional TiO2 hybridmicro/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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발표분야: 나노임프린팅 기술과 기능성 소재
발표종류: 심포지엄, 발표일시: 금 17:10, 좌장: 이승준

나노임프린팅 기술을 응용한 NWGP(nano-wire grid polarizer)Film 제조기술

허종욱

미래나노텍㈜

Room Temperature, Roll-to-Roll UV curable Nano-Imprinting 기술을 응용하여 LCD Back Light Unit 용도의 반사형 편광필름(Reflective polarizer film)을 제조하는 기술로서, NWGP film 의 광학 특성은 가시 광 영역에서 Tp, Rs 각각 over 45% 나타내며, 취급성, 내구성을 얻기 위해 그리드(grid) 표면에 보호층을 갖는 것을 특징으로 한다.

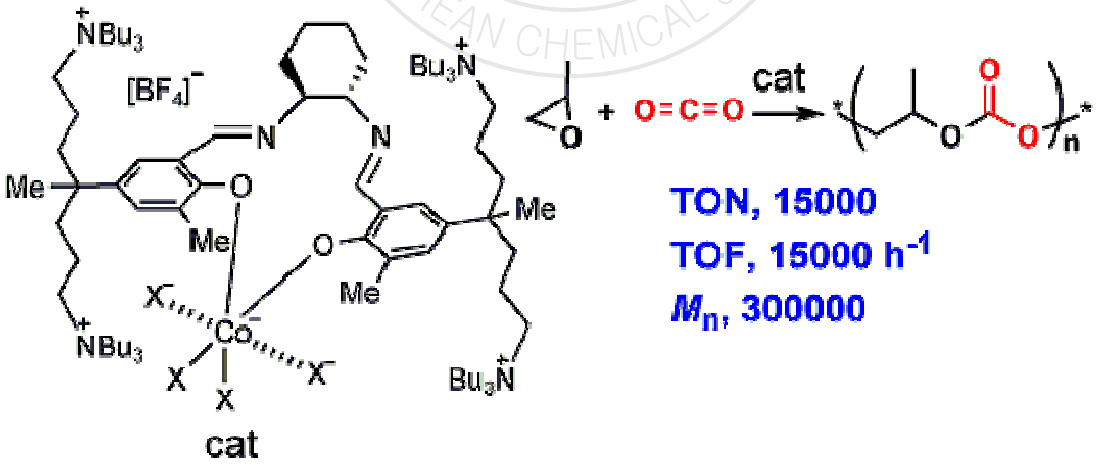
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND1-1**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 I
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 정민석

Converting CO_2 to a Valuable Polymer

이분열, Anish Cyriac

아주대 분자과학기술학과

A highly active catalyst was disclosed for the CO_2/propylene oxide (PO) copolymerization. It is a cobalt(III) complex prepared from a Salen-type ligand tethered by four quaternary ammonium salts, which adopts an unusual binding mode. The imine-nitrogens on the Salen-type ligand did not coordinate but, instead, the counter anions of the tethered quaternary ammonium coordinated to cobalt (1). Complex 1 showed a high TON up to 16000 and a high turnover frequency (TOF) of 16000 h^{-1} that produced a strictly alternating copolymer with a high molecular weight (Mn) of up to 300000. These performances of 1 allow for constructing a pilot plant for continuous commercial process.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND1-2**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 I
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 정민석

미세조류를 이용한 생물학적 이산화탄소의 고정화

심상준

성균관대 화학공학과

생물학적인 이산화탄소의 고정화는 속도가 늦은 반면에 유용물질로 전환되어 부가가치를 창출할 수 있다는 점에서 다른 방법에 비해 적극적이고 매력적인 요소를 가지고 있다. 이산화탄소를 고정화할 수 있는 생물은 식물이 대표적이며 그 이외에도 미세조류, 거대조류 등 광합성을 할 수 있는 생물과 이른바 chemoautotroph 와 같은 무기물을 이용하는 세균으로 나눌 수 있다. 결국 에너지원을 태양으로 하느냐 아니면 에너지준위가 높은 물질로 하느냐의 차이일 것이다. 최근 미국 유럽 등 선진국에서 특히 미세조류를 이용한 상업화 연구가 활발하게 이루어지고 있는 이유는 결국 이산화탄소의 고정화 속도가 상대적으로 빠르고 (식물의 15 배 이상) 바이오디젤 등 다양하고 유익한 유용물질의 생산이 가능하기 때문이다. 본 발표에서는 이산화탄소의 저감 필요성과 생물학적 이산화탄소의 특징 및 미세조류를 통한 이산화탄소 고정화 기술 사례 등을 토의해보고자 한다. 미세조류 반응 공정의 최적화, 광생물반응기 설계 시 고려사항 등도 논의해보기로 한다. 특히 현재 본 연구실에서 가동중인 광생물반응기의 개발과정과 옥외 배양 사례 발표 및 향후 거대 화력 발전소 실증 플랜트 설치 계획 등도 제시해 보고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND1-3**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 I
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 정민석

Biological Sequestration of Carbon Dioxide by Photosynthetic Microalgae

이철균

인하대

Algal biotechnology is drawing increasing interest due to its potential as a source of valuable pharmaceuticals, pigments, carbohydrates, and other fine chemicals. Its application has been extended to the areas of wastewater treatment and agriculture. Futhermore, recent development in various algal biotechnology found algal mass culture could be a useful solution in fixation of carbon dioxide, treatment of wastewater and production of biofuel.Green house gases such as CO_2 in the atmosphere became a serious problem for the whole mankind. The signs of global warming have boosted many researches on sequestration and removal of CO_2. One of the possible solutions is a biological CO_2 fixation using the photosynthesis of microalgae. Microalgal cultures don't need fresh nor clean water and they can grow on organic wastes and wastewaters (either municipal or livestock), while producing bioenergy or chemical feedstocks. However, the limitation of large scale cultivation and post-treatment of algal biomass hampers wide-spread use of microalgae for CO_2 reduction. Some of the current efforts of large-scale microalgal culture technology will be analyzed and compared.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND1-4**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 I
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 이분열

미세조류의 CO_2 고정화 및 biodiesel 생산 기술현황 및 전망

오희목

한국생명공학연구원 환경바이오연구센터

원유는 향후 50 년내에 고갈될 것으로 추정되는 한정된 자원이다. 또한 이와 같은 화석연료는 CO_2, SOx, NOx 등을 방출하여 지구온난화, 대기오염 등의 환경문제를 일으키고 있다. 따라서 전 세계적으로 대체에너지, 재생에너지 개발에 주력하고 있으며, 바이오에너지도 이에 속한다. 원유를 대체할 수 액상의 바이오에너지는 biodiesel 로 현재 콩, 옥수수 등의 작물로부터 주로 생산되고 있다. 광합성 미생물인 미세조류(microalgae)의 태양에너지 이용효율은 5%정도로, 육상식물의 0.2%에 비해 25 배 정도 높은 것으로 알려져 있다. 즉, 단위면적당 biodiesel 생산성이 높고, 비경작의 토지를 이용하는 장점이 있다. 현재 *Botryococcus* sp. *Pleurochrysis* 등의 미세조류를 이용한 biodiesel 생산이 시도되고 있다. 미세조류로부터 CO_2 고정 및 biodiesel 생산을 목표로 결성된 국제적 network 인 INMB (International Network for Microalgae Biofixation)의 목표는 2012 년까지 실현 가능한 기술개발로서 미세조류 생산성을 현재의 50 dw ton/ha/yr 로부터 2 배 수준이 100 dw ton/ha/yr 로 증대시키는 것이다. 장기적으로는 미세조류(*Botryococcus* sp.)의 배양면적을 점차 늘려 전 세계적으로 10 백만 ha 규모(전 세계적으로 운영되고 있는 새우와 물고기 양식장의 크기와 유사한 규모)의 pond 에서 미세조류를 배양하여 1 Gt 의 CO_2 방출 저감효과를 내는 것이다. 따라서 미세조류의 대량배양은 생물연료인 biodiesel 의 생산과 동시에 배양과정에서 대기 중 CO_2 의 흡수에 의한 지구온난화 방지효과를 동시에 달성할 수 있는 환경 친화적 에너지 생산기술이다. 그러나 미세조류 biodiesel 이 원유 diesel 과 경쟁하기 위해서 생산가를 현재의 $2.80/L 에서 $0.55/L 로 낮추어져야 한다. 미세조류로부터 biodiesel 생산의 경제성을 맞추기 위해 우선적으로 해결되어야 할 주요 기술분야는 1) 미세조류 탐색, 유전체 구조 및 기능 연구에 의한 우량 형질의 분자적 균주개량, 2) 미세조류 배양공정의 최적화, 광생물반응기(photobioreactor) 개발, 옥외 대량배양 등에 의한 고밀도 대량배양, 3) 특정

성분의 함량 증대를 위한 대사조절 및 biodiesel 의 효율적 생산을 위한 미세조류 수확법 개발, 4) 생산된 미세조류 biomass 를 biodiesel 로 전환하는 효율적이고, 경제적인 transesterification 공정개발 등이다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **IND1-5**

발표분야: 녹색공업화학: 이산화탄소 자원화 기술 I

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 이분열

이산화탄소를 활용한 유기카보네이트의 합성 및 활용

이현주

KIST 청정에너지연구센터

이산화탄소는 지구온난화의 주요 원인 물질로 규정되어 최근 분리, 배출, 그리고 저장에 관련된 기술이 활발하게 연구되고 있다. 그러나 다른 한편으로는 독성이 없을 뿐만 아니라 지구상에 풍부하게 존재한다는 점에서 친환경적인 화합물이기도 하다. 유기카보네이트는 이산화탄소가 화학적으로 변형된 상태이다. 이들은 그 자체가 반응 용매, 전해질 용매 등으로 실제 적용되고 있을 뿐만 아니라 기존의 독성 할로겐 화합물, 대표적으로 포스겐을 대체할 수 있는 원료로 사용되고 있다. 실제로 아직도 많은 양의 폴리카보네이트가 포스겐으로부터 제조되고 있지만 이산화탄소를 원료로 하는 디페닐카보네이트를 사용하여 제조되는 방법이 점차 그 점유율을 높여가고 있다. 알킬렌카보네이트나 디알킬 카보네이트, 카바메이트 그리고 유레아 등도 이산화탄소로부터 직접/간접적으로 제조할 수 있는 방법이 이미 다양하게 개발되어 있고 일부는 상용화되어 있다. 본 발표에서는 유기카보네이트와 관련된 최근 연구동향을 살펴보고 특히 최근 연구가 집중되고 있는 글리세롤카보네이트의 합성과 활용에 대하여 살펴보겠다.

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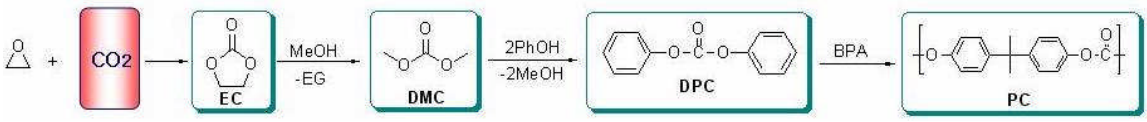
장소: 대구엑스코
발표코드: **IND2-1**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 13:00, 좌장: 정광덕

이산화 탄소 활용을 통한 폴리카보네이트 제조 기술

권오성, *장복남, **지준호, ***허종찬

*제일모직(주) 케미칼연구소 *제일모직 케미칼 연구소 **제일모직 케미칼연구소 ***제일모직 (주) 케미칼연구소 PC그룹*

교토의정서 발효 이후 이산화탄소(CO2)에 감소에 대한 관심은 크게 증가하고 있으며 이에 따라 이산화탄소 감소에 대한 연구도 활발히 진행되고 있다.이산화탄소의 화학적 재활용 기술은 탄소세 등의 환경세 도입시 발생되는 제품의 원가상승 억제 및 에너지 및 화학제품의 원료로서의 응용을 가능하게 함으로써 새로운 이윤창출의 기회로 활용될 수 있기에 많은 기업들의 관심이 대상이 되고 있다.우수한 특성으로 인하여 활용 범위가 지속적으로 증가하고 있는 엔지니어링 플라스틱의 하나인 폴리카보네이트는 이산화탄소를 원료로하여 제조할 수 있으며, 이 제조 기술은 환경친화적이며 제조되는 폴리카보네이트 무게의 약 22%에 해당하는 이산화탄소를 원료로 사용하는 매력으로 인하여 매우 빠르게 확산되고 있는 화학적 재활용 기술이다. 본 발표에서는 이산화탄소를 활용한 폴리카보네이트의 제조 및 현황에 대해 고찰하고자 한다.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND2-2**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 정광덕

제철산업에서의 이산화탄소 포집 및 자원화 기술개발

전희동

(재)포항산업과학연구원 CO2 연구단

이산화탄소의 대기 배출을 줄이기 위한 실제적 수단으로서 이산화탄소 포집 및 저장(CCS) 기술은 대단히 중요하며 우리나라도 최근 이 분야에 기술개발을 집중하고 있다. 그러나 저장에 대한 세계 각국의 현실을 살펴보면 저장지가 충분한 나라를 제외하고는 실현 가능성에 회의적인 시각이 상당하며 저장 그 자체에 비용도 상당하다. 따라서 어렵게 포집한 이산화탄소를 단순히 저장하는 것 보다 자원으로 이용하고자 하는 시도는 매우 의미가 있다. 그러나 이산화탄소를 자원화하기 위해서는 이산화탄소를 일단 반응성이 있는 일산화탄소 등으로 전환하는 것이 필요하며 여기에는 수소나 메탄 등의 환원제와 높은 에너지가 필요하다. 일반적으로는 환원제를 얻는 과정이나 높은 에너지를 공급하는 과정에서 이산화탄소를 배출하게 되므로 대부분의 이산화탄소 자원화하는 기술은 실제 이산화탄소 저감효과를 얻기가 어렵다. 반면 제철산업에서는 공정의 특성 상 환원제로 사용할 수 있는 다량의 메탄과 고온의 폐열을 부산물로 얻을 수 있으므로 실제 이산화탄소를 저감하는 좋은 자원화 사례가 될 수 있다. 당 연구단에서는 포항제철소에서 이산화탄소를 포집, 일산화탄소로 환원하여 이를 고로에서 철광석 환원제로 사용하기 위한 연구를 지난 2009 년부터 지식경제부 연구과제로 진행 중이다. 본 발표에서는 제철산업에서의 이산화탄소 포집기술 개발현황과 이를 일산화탄소로 환원하기 위한 폐열회수기술, 촉매환원기술 등 요소기술 개발 내용과 주요 성과 및 향후계획 등을 소개하고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND2-3**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 정광덕

SK energy's New CO2-Embeded Polymer Technology: GreenPol™

옥명안

SK에너지 기술원 화학연구소

SK energy (SKE) has entered into the new world of sustainable plastics by introducing its proprietary CO2-embeded polymer technology, GreenPol™, an alternating copolymer of CO2 and epoxides. Major advantages are CO2 utilization to valuable materials and low petroleum dependency. Whole production process shows the lowest CO2 emission among existing commodity polymers. Polymer itself is also an eco-friendly material with various useful properties: clean burning, barrier properties to O2 and H2O, enzyme degradability, transparency, printability, adherence, etc. Thanks to these properties, GreenPol™ is applicable to various fields: insulating/shock absorbing material, upholstery, packaging, adhesives, coating, etc. GreenPol™ technology is composed of catalyst, process and product technology. SKE has already developed world best catalyst and process technology, has been developing suitable applications and is making a lot of efforts to expand its applicability and marketability.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND2-4**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 옥명안

일 10톤 DME 생산플랜트 기술개발

조원준

한국가스공사 연구개발원 DME연구개발

차세대 청정연료로 각광을 받고 있는 DME 는 청정성이 LPG 와 유사하여 LPG 와 혼합하여 혼합연료로 활용할 수 있으며 세탄가가 디젤연료와 유사하여 디젤연료를 대체할 수 있는 청정에너지이다. 이러한 DME 를 생산하기 위하여 한국가스공사에서는 기존의 메탄올로부터 DME 를 생산하는 간접합성방법이 아닌 다양한 원료가스 즉, 천연가스, CBM, Biomass 등으로부터 DME 를 직접 합성하는 직접합성법을 세계 4 번째로 개발하였다. 이 직접합성법의 가장 큰 특징은 원료가스로 CO_2 를 활용하여 DME 합성을 위한 합성가스를 제조하는 것이다. 따라서 CO_2 를 포함하고 있어 상대적으로 경제성이 떨어지는 가스전을 개발하여 DME 를 제조하면 경제성을 확보할 수 있다. 한국가스공사에서 개발한 DME 생산 플랜트는 크게 4 개의 공정으로 구성되어 있다. 먼저 첫 번째로 원료가스를 공급하여 삼중개질반응기에서 H2 와 CO 로 이루어진 합성가스를 제조하는 Syngas section, 그리고 두 번째로 합성가스 제조시 부산물로 생성되는 CO_2 를 분리하여 다시 원료가스로 재활용하는 CO_2 removal section, 세 번째로 CO_2 가 분리된 합성가스로부터 DME 를 합성하는 DME synthesis section, 마지막으로 합성된 DME 를 분리 정제하여 고순도의 DME 로 저장하는 DME purification section 으로 구성된다. DME 합성을 위하여 생성되는 합성가스는 H_2/CO ratio 가 이론적으로 1.0 에 가까울수록 DME 합성에 최적의 합성가스 비율을 나타낸다. 따라서 본 공정에서 합성가스 비율이 1.0 에 가깝게 생산하기 위하여 메탄가스를 O_2, steam 그리고 CO_2 를 활용하여 합성가스를 제조하는 삼중개질반응기(Tri-reformer)를 개발하였다. Tri-reformer 는 합성가스 비율을 4.0 에서 1.0 까지 다양하게 제조할 수 있는 것이 특징이다. DME 합성을 위한 DME 합성 반응기는 DME 합성시 발생하는 발열을 효과적으로 제거하는 제열시스템을 개발하여 적용하였다. 이를 통하여 DME 합성반응 온도를 약 230~280℃로 제어가 가능하여 효과적으로 DME 를 합성할 수 있다.

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장소: 대구엑스코
발표코드: **IND2-5**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 옥명안

이산화탄소저감 메탄올 제조촉매 및 공정기술 CAMERE-II

정광덕

KIST, 청정에너지센터

상업적으로 메탄올은 메탄의 스팀리포밍에 의해 합성가스를 생산하고 이를 활용하여 메탄올을 합성하는 2 단계 반응으로 구성된다. 메탄의 스팀리포밍반응은 R ratio ((H_2-CO_2)/(CO+CO_2))가 3.0 으로 과량의 수소가 발생하고 상용화공정에서는 이러한 수소를 메탄리포밍의 열원으로 사용하게 된다. ICI 공정에서는 이산화탄소를 리포머에 도입하거나 메탄올반응기에 도입하여 약 5-8%의 경제성이 향상되는 것으로 보고되고 있다. 한국과학기술연구원에서는 역수성가스반응촉매/반응시스템을 기존의 메탄올합성공정에 도입하고 이산화탄소를 역수성가스반응기에 공급하여 R ratio 가 2.0 이 되도록 조정함으로써 메탄대비 메탄올의 수율을 120%이상 달성하는 것이 가능한 공정을 개발하였다 (CAMERE-II). 메탄올합성촉매는 $Cu/ZnO/Al_2O_3$ 촉매를 사용하였다. 이 반응은 structure insensitive reaction 으로 메탄올 합성의 반응성은 구리의 표면적에 비례하여 높은 Cu 표면적을 갖는 Cu/ZnO 기반 촉매를 합성하는 것이 중요하였다. 역수성가스반응은 600 oC 이상의 고온의 환원가스하에서의 반응으로 상용화된 수성가스촉매는 촉매의 환원 및 탄소침적으로 비활성화가 심하여 ZnO 기반의 촉매가 가장 좋은 활성 및 안정성을 나타내었다. 본 심포지엄에서는 이산화탄소 저감을 위한 메탄올/DME 합성공정인 CAMERE-II 공정 및 CAMERE-II 공정에 관련한 촉매의 합성방법 및 반응기구에 대해 논의 하도록 하겠다.

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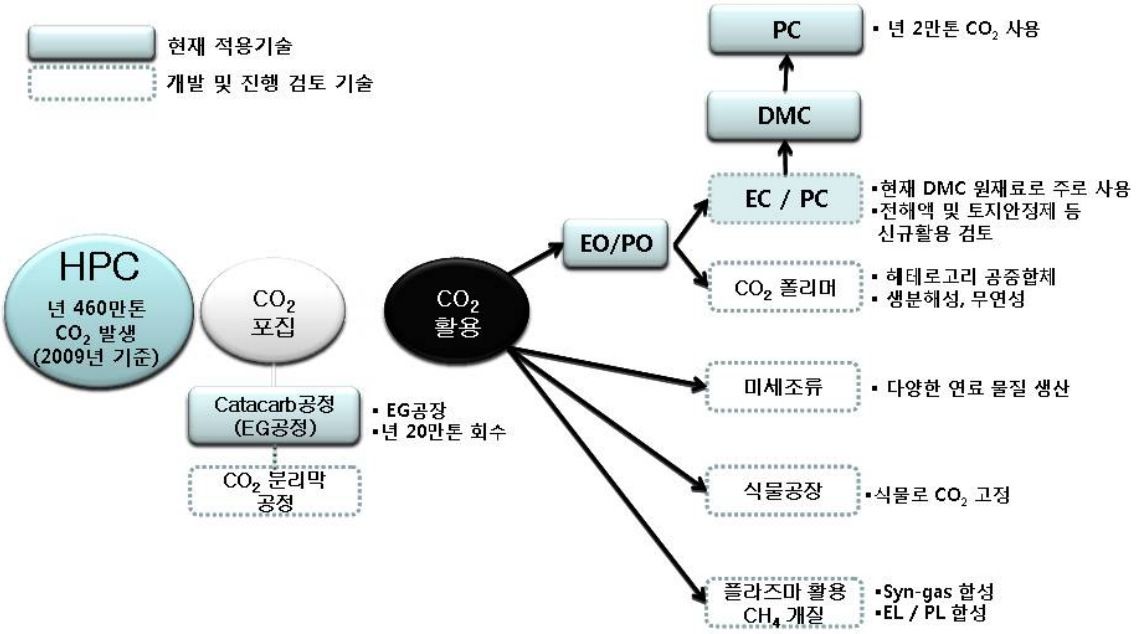
발표코드: **IND2-6**
발표분야: 녹색공업화학: 이산화탄소 자원화 기술 II
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 옥명안

호남석유화학의 이산화탄소 활용 및 연구 방향

김창규

호남석유화학(주) 소장실

호남석유화학에서는 현재 연간 460 만톤의 이산화탄소가 발생하고 있으며, 이런 이산화탄소를 회수 및 활용하기 위한 방안은 다각적으로 모색하고 있다. 현재는 알칼리수용액을 이용한 카타카브시스템으로 이산화탄소를 회수하고, 그 회수된 이산화탄소는 폴리카보네이트 합성에 이용하고 있다. 최근에는 분리막을 이용하여 LNG 보일러로부터 이산화탄소를 분리하는 기술을 개발 중에 있고 회수된 이산화탄소를 자원화 위해 다양한 연구를 하고 있다. LNG 보일러 배기가스로 부터 이산화탄소를 회수하여 식물에 적용하는 친환경 식물공장 시스템, 미세조류에 이산화탄소를 고정시켜 바이오디젤이나 기타 유용물질로 전환하는 연구, 메탄과 이산화탄소를 플라즈마로 이용하여 합성가스로 개질하는 연구, 새로운 이산화탄소 폴리머, 고부가가치인 EC, PC 사업 등 본격적으로 이산화탄소 회수 및 활용 연구를 진행하려고 한다.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR1-1**
발표분야: 에너지변환 광동력학
발표종류: 분과기념강연, 발표일시: 금 09:00, 좌장: 김진홍

Self-crystallization of fullerene

최희철

포항공과대 화학과

Fullerene is a representative highly conjugated molecular system of which electronic configuration is well defined to behave as a semiconductor and superconductor when properly doped. To extend its vulnerability, geometrically well-defined structures are highly demanded not just for handling them easily during fabrication into electrical devices, but more importantly for modulation of their electrical or optical properties by defining how their neighborhood molecules are positioned. Self-crystallization is a powerful process that allows high definition single crystalline fullerene structures with high specificity in 1D, 2D, and 3D geometries. In this presentation, I will introduce two self-crystallization processes in vapor and solution phases that have successfully resulted in hexagonal C60 disks and wires, as well as C70 cubes. For the hexagonal C60 disks, a simple vaporization-condensation-recrystallization (VCR) process has been employed, and similar C60 disks and wires have been selectively obtained by choosing appropriate solvents in drop-drying process. In the case of C70 molecules, they are spontaneously self-crystallized into very homogeneous cube crystals by a simple precipitation process employing good solvent microcavities in poor solvent media. Together with the detail story of synthesis and structure characterizations, dramatic enhancement of photoluminescence property of C70 cubes will be also introduced.

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장소: 대구엑스코
발표코드: **INOR1-2**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 박강현

Photoinduced Electron Transfer in Heteroleptic Ir(III) Complexes with Light-Harvesting Carbazole dendrimers

조대원

고려대 신소재화학과

We synthesized a heteroleptic Ir(III) complex and a series of its dendrimer systems. We investigated their photophysical properties, coupled with photodynamic behavior, to explore possible photo-functionalities of the dendrimers. Transient-spectroscopic studies demonstrated that phosphorescence quenching in Ir-dendrimers occurs by efficient electron transfer from the excited carbazole (Cz) unit to the core ligands, and that the electron-transfer efficiency decreases with the increase in dendrimer generation associated with an increase in distance between the donor-acceptor pair. Selective excitation of the carbazole units resulted in fluorescence quenching of excited Cz due to energy transfer to the Ir-complex core. The fluorescence quenching efficiencies of Cz were determined to >90% on the basis of steady-state fluorescence spectra and the decay time constants. The reduced quenching efficiencies of Cz in high-generation dendrimers are probably attributable to the long distance between Cz dendrons and the Ir-complex core. The photoluminescence from the ^{3}MLCT state is enhanced with increasing numbers of Cz dendron units. However, actual enhancement of photoluminescence from the Ir complexes was low because the ^{3}MLCT emission was quenched by photoinduced electron transfer (PET) from Cz to Ir metal ions. We probed the Cz cation radical species generated by PET in the ^{3}MLCT state by examining the transient absorption.

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장소: 대구엑스코
발표코드: **INOR1-3**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박강현

Energy transfer dynamics in OLED devices

송재규

경희대 화학과

The energy transfer dynamics in organic light emitting diode (OLED) is studied. The doping of phosphorescent sensitizer (Ir(ppy)3) in the well-known hole transport layer (HTL, m-MTDATA) induces the energy transfer between m-MTDATA and Ir(ppy)3. The energy transfer from m-MTDATA to Ir(ppy)3 is observed in nanosecond regime along with the energy transfer from Ir(ppy)3 to m-MTDATA in a few hundred nanosecond regime, which enhances the phosphorescence of m-MTDATA. In addition, the doping of another phosphorescent sensitizer (FIpic) is found to facilitate the phosphorescence of m-MTDATA more effectivley due to the reasonably matched energy levels between them.

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발표코드: **INOR1-4**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 박강현

Unique Photo-electronic Properties of Mesoporous TiO_2 Single Nanofiber Including Au Quantum Dot

김용록, 임지은, 왕강균, 오승임, 김봉진, 신언필, 민경명

연세대 화학과

In this work, fabrication of mesoporous TiO_2 single nanofiber (MTSN) composites is reported and their various applications are discussed in the aspects of electronic, optical, and opto-electronic factors. The MTSNs are fabricated by using sol-gel method within the nanochannels of porous alumina membrane. Due to the large surface area and photoconductivity, the MTSNs are investigated for the applications of gas and UV sensors. The synthesized MTSNs are loaded with Au nanoparticles through pores of MTSN by a deposition-precipitation method. Upon irradiation with visible light, the MTSN loaded with Au nanoparticles (MTSN-Au) exhibits wavelength-dependent and reversible photoresponse which is induced by the surface plasmon resonance absorption. In addition, we investigate the effects of the Au nanoparticles on electronic transport properties of the MTSN-Au nanofibers. This study shows that utilization of surface plasmon resonance of Au nanoparticles can be a method for improvement of the photoconversion efficiency of solar cell.

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장소: 대구엑스코
발표코드: **INOR1-5**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 옥강민

Molecular Structure and Chemical Reaction: Physical Chemist's view

김상규

KAIST 화학과

Moecular structure and its relation to chemical reaction have been the essential topic for last decades. In many areas of chemistry, chemists always tend to understand chemical phenomena based on the structure of the molecule involved in such processes. In many cases, Although there are many successful examples in such endeavor, the detailed relation of the structure and chemical-reactivity seems to be still in infancy. In this talk, the approach of a physical chemist to this problem will be introduced and discussed.

THE KOREAN CHEMICAL SOCIETY

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장소: 대구엑스코
발표코드: **INOR1-6**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 옥강민

Photodynamic Studies of TiO_2-Nanostructure Composites toward Solar Energy Conversion Systems

윤민중

충남대 화학과

TiO_2 nanomaterials are of great current interest for applications in photo-electronic materials including light-energy conversion, artificial photosynthetic systems as well as photocatalysis. The success of these applications relies on the exciton recombination dynamics and visible-light sensitivity of the TiO_2nanomaterials. Thus, in order to develop the highly efficient photo-electronic materials absorbing visible light, different low dimensional visible-light sensitive TiO_2nanostructures such as nanodiscs, nanofibers and N-doped nanochains were synthesized by sol-gel and/or hydrothermal methods, and thereafter their surfaces were further modified by incorporating with heteropoly tungstic acid($H_3PW_{12}O_{40}$) (HPA), Sn-porphyrins, or silver ion. The optical properties and the surface exciton dynamics of the surface-modified nanomaterials were investigated using both ensemble and single nanoparticle photoluminescence techniques. These results were correlated with the photocatalytic activities and solar cell efficiencies, indicating that the electron transfer mechanism in the modified nanostructures may be similar to the "Z-scheme" of the plant photosynthetic system so that both photocatalytic activity and solar cell efficiencies were synergistically enhanced. References:Yoon, M.; Chang, J. A.; Kim, Y.; Lee, S. I.; Kim, K. *J. Phys. Chem. B* 2001, *94*, 2539Yoon, M.; Seo, M.; Jeong, C.J.; Jang, H.; Jeon, K.S. *Chem. Mater.* 2005, *17*, 6069 Jeon, K.S. ; Yoon, M. et al., *Phys. Chem. Chem. Phys*. 2009, *41*, 534Parayil, S. K.; Lee, Y. M.; Yoon, M. *Electrochem. Comm*. 2009, *11*, 1211 Lee, J.; Lee, Y.-H; Yoon, M. *ACS Nano* 2010 submitted

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR1-7**
발표분야: 에너지변환 광동력학
발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: 옥강민

Interfacial Electron Transfer in Quantum Dot Modified with Pyromellitimide

Tetsuro Majima

Institute of Scientific and Industrial Research, Osaka University

Photoinduced electron transfer (ET) to and from semiconductor quantum dots (QDs) is of intense interest because of its important roles in QD-based devices, such as detectors, light-emitting diodes, and solar cells. We have investigated the interfacial ET between CdTe QDs or ZnS-capped CdSe (CdSe/ZnS) QDs and pyromellitimide (PI) at the ensemble and single-particle levels. $PI^{\bullet-}$ is generated by the ET with photoexcited QDs. The single-particle PL imaging reveals that the apparent number of luminescent QDs decreased by the conjugation with PI derivative with a carboxylic acid (PI-CA). The blinking characteristics with and without PI-CA was rationalized in terms of the diffusion-controlled ET (DCET) theory. We proposed the intermittent ET mechanism for the charge separation and recombination dynamics between the CdTe/PI-CA where the temporal fluctuations in local environments, adsorbate conformation, and vibronic coupling, play key roles. The solvent dependence of the ET between CdSe/ZnS QDs and PI-CA. It was found that two pathways are included in the ET processes from the excited CdSe core and ZnS to PI-CA molecules, on ps and ns time scales, respectively. The PL intermittency or blinking kinetics of single QDs analyzed by the DCET theory showed that the ET probability increases with the decreasing solvent polarity. Consequently, our findings provide new insight into the mechanism of the ET on the semiconductor nanoparticles and potentially contribute to the development of design of QD-based devices.

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장소: 대구엑스코
발표코드: **INOR2-1**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 허남회

Metal Nanocrystal Synthesis: Past, Present, and Future

Younan Xia

Washington University

The first documented synthesis of colloidal nanocrystals can be traced back to the beautiful work by Michael Faraday in 1856 when he demonstrated the preparation of gold colloids with a ruby-red color. However, only within the last decade have chemical methods been developed for generating nanocrystals in the quality, quantity, and reproducibility required for a systematic study on their properties as a function of size, shape, and structure. I will briefly cover some of these developments in this a talk, with a focus on shape-controlled synthesis of noble-metal nanocrystals. Part of our research over the last decade has focused on shape-controlled synthesis in solution phase. While the synthetic methodology mainly involves solution-phase redox chemistry, we have been working diligently to understand the complex physics behind the simple chemistry – that is, the nucleation and growth mechanisms leading to the formation of nanocrystals with specific shapes. We discovered that the shape of silver nanocrystals are dictated by both the crystallinity and shape of nanocrystallite seeds, which are, in turn, controlled by factors such as reduction rate, oxidative etching, and surface capping. The same mechanism also works for other noble metals including gold, palladium, platinum, and rhodium. The success of these syntheses has enabled us to tailor the electronic, plasmonic, and catalytic properties of noble-metal nanocrystals for a range of applications.

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장소: 대구엑스코
발표코드: **INOR2-2**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 허남회

Chemical Design of Nanoparticles for Bio-Medical Applications

천진우

연세대 화학과

Magnetic nanoparticles that exhibit a variety of unique nanoscale phenomena are garnering significant interest since nanoscale properties can be leveraged in their utilization as probes and vectors for novel biomedical applications. Here, we discuss the nano-scaling laws of magnetic nanoparticles including metals, metal ferrites, and metal alloys with focuses on their size, shape, and composition effects. Such scaling laws are found to be critical to design magnetism characteristics of nanoparticles for their enhanced applicability in biomedical sciences including magnetic resonance imaging (MRI), nano-bio hybrids, and magnetophoretic sensing of biological targets. We have successfully demonstrated such high-performance nanotechnology-based materials could enhance the ability to characteristics critical to diagnostics and therapeutics.

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장소: 대구엑스코
발표코드: **INOR2-3**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 허남회

Nanocrystal Solids: A Modular Approach to Materials Design

Dmitri Talapin

University of Chicago

Colloidal nanocrystals can combine the advantages of crystalline inorganic semiconductors with size-tunable electronic structure and inexpensive solution-based device fabrication. Single- and multicomponent nanocrystal assemblies, also known as superlattices, provide a powerful general platform for designing two- and three-dimensional solids with tailored electronic, magnetic, and optical properties. Unlike atomic and molecular crystals where atoms, lattice geometry, and interatomic distances are fixed entities, the nanocrystal arrays represent ensembles of "designer atoms" with potential for tuning their electronic structure and transport properties. Generally speaking, nanocrystal assemblies can be considered as a novel type of condensed matter, whose behavior depends both on the properties of the individual building blocks and on the interparticle exchange interactions. The ability to assemble precisely engineered nanostructures into complex structures is opening the door to a new generation of materials where components and functionalities can be added, tuned or combined in a predictable manner. I will show how self-assembly of nanocrystals can lead to a palette of unprecedented phases including superlattices isostructural with the Archimedean tilings and dodecagonal quasicrystals. The facile charge transport is crucial for performance of nanocrystal-based electronic and optoelectronic devices. The insulating nature of the surface ligands used for nanocrystal synthesis typically results in the poor electronic coupling between individual nanocrystals. To address this fundamental problem, we demonstrate that molecular metal chalcogenide complexes can serve as versatile ligands for a broad range of inorganic nanomaterials. I will demonstrate the power of this approach on several examples of prospective electronic, thermoelectric and photovoltaic materials.

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장소: 대구엑스코
발표코드: **INOR2-4**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 천진우

Designed Assembly of Uniform-sized Magnetite Nanocrystals for Multifunctional Biomedical Applications

현택환, 이지은, 이노현, 김병효, 박미현

서울대 화학생물공학부

Clever combination of different nanoscale materials will lead to the development of multifunctional nano-biomedical platforms for simultaneous targeted delivery, fast diagnosis, and efficient therapy. In this presentation, I would like to present some of our group's recent results on the designed fabrication of multifunctional nanostructured materials based on uniform-sized magnetite nanoparticles and their bio-medical applications. We fabricated monodisperse magnetite nanoparticles embedded in uniform pore-sized mesoporous silica spheres and PLGA polymers for simultaneous MRI, fluorescence imaging, and drug delivery. We synthesized highly versatile nanocomposite nanoparticles by decorating surface of mesoporous dye-doped silica nanoparticles with multiple magnetite nanocrystals, and we demonstrated in vivo passive targeting and accumulation of the nanoparticles at the tumor site confirmed by both T2 MR and fluorescence imaging. We used uniform ferrimagnetic magnetite nanocrystals for T2 MRI contrast agent for tracking transplanted pancreatic islet cells. We synthesized hollow magnetite nanocapsules and used them for both MRI contrast agent and magnetic guided drug delivery vehicle.

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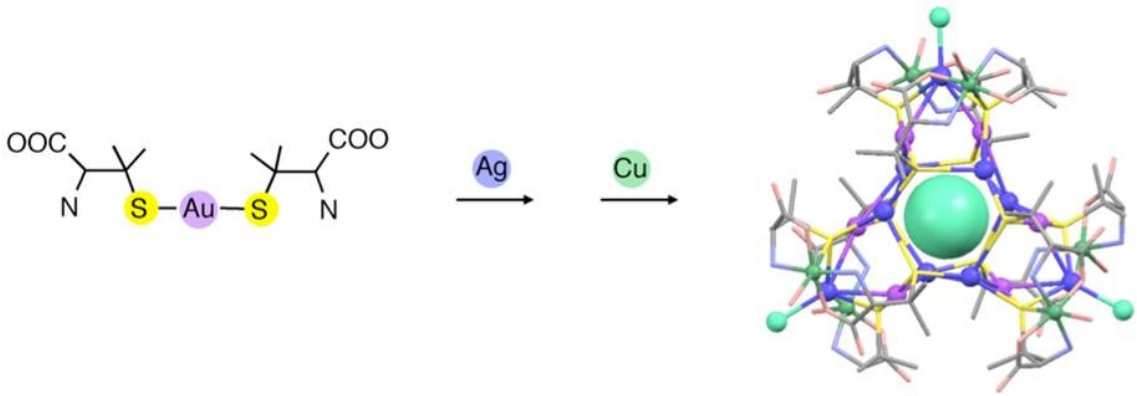
발표코드: **INOR2-5**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 천진우

D-Penicillaminato Metalloligand Systems That Lead to a Variety of Chiral Heterometallic Aggregates

Takumi Konno

Osaka University, Japan

While a large number of metalloaggregates have been synthesized through the self-assembly of multidentate organic ligands assisted by metal ions, our synthetic strategy has been directed toward the use of metal complexes with thiol-containing amino-acids, such as L-cysteine (L-H_2cys) and D-penicillamine (D-H_2pen), as a functional metalloligand. Here we present the rational construction of chiral heterometallic aggregates based on a two-coordinate Au^I metalloligand, $[Au(D\text{-}pen)_2]^{3-}$, which possesses two amine and two carboxylate groups as potential coordination sites, besides two coordinated thiolato groups. Another metalloligand system will also be presented.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR2-6**
발표분야: 무기 나노 재료의 발전 방향
발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 천진우

Porous Coordination Polymers for Hydrogen Storage and Carbon Dioxide Capture

백명현

서울대 화학부

Porous coordination polymers (PCPs) have attracted great attention as new functional materials. We have constructed various types of PCPs from the self-assembly of metal and organic building blocks. We have increased the H_2 storage capacities of PCPs by creating greater surface area, incorporating functional groups in the ligand, generating vacant coordination sites on the metal ions, and embedding Pd nanoparticles in the PCP channels. We have achieved highly selective CO_2 capture by constructing flexible 3D networks that open and close their gates depending on the CO_2 pressure while not responding to other gases. The post-synthetic insertion of an appropriate bridging linker in a porous network also leads to the selective CO_2 capture.

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발표코드: **PHYS1-1**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이진용

Volume, Statistical Mechanics, and Molecular Representation of Molar Volume

Byung Chan Eu

McGill University, Canada

In this talk, the concept of volume in matter, and in particular, the molar volume in condensed matter, will be discussed from the thermodynamic and molecular theory viewpoints. According to statistical mechanics, thermodynamic observables, such as density, energy, pressure, entropy, heat, etc. are possible to compute directly from their molecular (atomic) theory definitions such as mass, Hamiltonian (e.g., kinetic energy + potential energy), Clausius's virial, work, etc., by taking an ensemble of particles (atoms or molecules) in a container of volume V and averaging their evolution in time or in the phase space of particles. With a suitable thermodynamic correspondence scheme between the thermodynamic and mechanical quantities we acquire a molecular theory of matter, which is called statistical mechanics, underlying our current understanding of the behavior and properties of macroscopic matter (gas, liquid, or solid). However, molar volume is unique among all macroscopic observables in that it has not enjoyed a molecular theory definition, because it is hitherto unknown how one might directly compute it by using the method of statistical mechanics on the basis of its molecular theoretic representation. It will be discussed how we may achieve the goal of obtaining a molecular representation of molar volume by using the notion of Voronoi polyhedra in analogy to the Wigner--Seitz cell in solid state physics. The implications of the thus-obtained notion of molar volume in molecular theory will be discussed in connection with fluid dynamics. For example, the mean Voronoi volume---the molar volume---gives rise to the necessity of generalizing the conventional hydrodynamics, namely, Navier--Stokes--Fourier--Ficks hydrodynamics, because the mean Voronoi volume is not a collision invariant unlike density, momentum, energy, angular momentum and thus qualifies as a non-conserved variable in the same rank as stress tensors, heat fluxes, diffusion fluxes, etc. which are directly involved in the energy dissipation in transport processes. Simply put, it compels a paradigm change in fluid dynamics and presents a new vista to the

theory of transport in fluids. It also broadens our modes of thinking in condensed matter physics and chemistry. It helps us better understand the space per particle in condensed phase.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PHYS1-2**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이태걸

Polymer nanotechnology for optical imaging

권익찬

KIST 의과학센터

In recent years, advances in medical imaging technology have been emphasized along with new advances in the field of cellular and molecular biology. Emerging field of medical imaging, i.e. Molecular Imaging, allows not a traditional image of anatomical changes, but a biological characterization of disease state at molecular or cellular lever. Interdisciplinary research at the interface of nanotechnology and molecular imaging had led to elucidate key factors that determine specificity in diagnosis and therapeutics. For example, with combining molecular imaging technology and drug delivery system, a novel design of drug screening or new approaches in drug development can be performed in animal models. Polymer nanoparticles bearing near-infrared fluorescent dyes can be utilized in determining optimized therapeutic dosages or frequencies of drug administration. These nanoparticles also can be utilized as molecular probes for visualization of therapeutic efficacy in small animals. Design of novel polymeric nanoparticles with high specificity in cellular or molecular responses, application of molecular imaging probes toward the era of Personalized Medicine will be presented in current study

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발표코드: **PHYS1-3**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이태걸

Fluorescence-SERS Dual Modal Nanoprobes: Application to Molecular Imaging of Cancer Cells Expressing Multiplex Biomarkers

주재범

한양대 생명나노공학과

We report a highly sensitive optical imaging technology using dual-modal metal nanoparticles for cellular imaging or biomedical diagnostics. Fluorescence microscopy is a well-known imaging technique which provides a specific protein distribution inside cells. However, most of currently available fluorescent organic dyes have relatively weak emission intensities and they are also photo-bleached quickly. In order to resolve this problem, more sensitive and stable probes are still needed. In the present work, dual modal nanopronbes, which can be used for both the Surface-enhanced Raman scattering (SERS) and fluorescence detections, have been developed. SERS detection is a powerful analytical technique that allows ultra-sensitive chemical or biochemical analysis in terms of unlimited multiplexing and single molecule sensitivity. Combining advantages of fluorescence and SERS allow these dual modal nanostructures to be used as powerful probes for a novel biomedical imaging. In this presentation, the synthesis and characterization of the fluorescence-SERS dual modal nanoprobes and their biological imaging application will be presented.

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장소: 대구엑스코
발표코드: **PHYS1-4**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이태걸

Multiplex coherent anti-Stokes Raman scattering microscopy for fast imaging and spectroscopic analysis of lipid-rich structures

이재용

한국표준과학연구원 미래융합기술부

Coherent anti-Stokes Raman scattering (CARS) has received considerable attention in the field of label-free biomedical imaging, for its high sensitivity to molecular vibrations offering inherent chemical contrast. However, current implementations of CARS microscopy mostly depend on the monochromatic image contrast designated by a single Raman shift and often require more detailed vibrational information to be obtained for high molecular specificity. We present 3-color multiplex CARS microscopy in which a femtosecond broadband laser is used as a pump beam. The CARS imaging platform facilitates a prompt recording of broadband CARS spectra along with a fast CARS microscopy. Employing a 3-color multiplex CARS scheme, we are able to incorporate a commercially-available, power-abundant femtosecond laser as a broadband pump beam, with the aid of separate picosecond Stokes and probe beams being introduced in the near IR. Experimentally, high-resolution multiplex CARS signals are allowed to investigate molecular vibrations in the range of 2600 cm^{-1} – 3100 cm^{-1}, which are found to be also useful to construct lipid-sensitive images with high signal-to-noise ratio (> 10:1). It is demonstrated that the proposed implementation promises a particular benefit on CARS imaging of lipid-rich tissue structures by providing detailed information on -CH_n Raman-active vibrations at a point of interest (POI) on the CARS images that can be obtained at high frame rates (> 1 frame/s). A label-free, nondestructive, 3-D, en-face vibrational histology of atherosclerotic plaques and multiplex spectral analysis are performed concurrently in mouse cardiovascular tissues.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PHYS1-5**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 주재범

Design and Synthesis of Nanostructured Materials for Biomedical Imaging and Therapy

정봉현

한국생명공학연구원

Recently, the creation of nanostructured materials has substantially influenced many areas including biology and medicine. Nanomaterials are also expected to be the core technology in the area of nanomedicine. that will lead the future technology trend. Recently, many researchers are focusing on the development of nanomaterials that can diagnose and treat cancer at the same time, by combining imaging agents, targeting antibody and therapeutic moieties. This lecture will focus on our rational design of so-called “smart nanomaterials” with multifunctionality, and their potential applications for biomedical imaging and therapy. In addition, a variety of nanostructured materials developed in our laboratory will also be discussed in terms of practical applicability.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표코드: **PHYS1-6**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 주재범

Nanomedical Technology in Personalized Cancer Medicine

허용민

연세대 의료원

In vivo understanding of target molecules via molecular imaging with nanoprobe is crucial to assess indication of targeted drug and to monitor its efficacy in patients, which are the key factors in planning personalized cancer therapies. In the smart contrast agent, target contents is the cornerstone to cataloguing patient subgroups and evaluating targeted anticancer drug efficacy as well as its resistance. Further, the ultrasensitivity from high crystallized monodiverse metal oxide nanoparticle enables us to image very small sized tumor via MRI. On the other hand, in vitro measurement of target contents has a critical role to optimize personalized cancer medicine. These contents promise various nanoplatforms and nanodevices to translate precise and sensitive nanobiosensor into personalized clinical settings. Thus it is necessary to develop in vivo and in vitro diagnostic tools to measure multiple targets and/or signaling pathways of cancer toward personalized medicine.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **PHYS1-7**
발표분야: 바이오메디컬 이미징 기술
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 주재범

An Ionic liquid matrix for MALDI Imaging Mass Spectrometry of Phospholipids

김광표

건국대 분자생명공학과

Phospholipids are the major building block molecules of cellular membranes. Information regarding phospholipid distribution in tissue has important physiological and pathological significance. Because the concentration of phospholipids changes in different disease states, assessment of the phospholipid distribution is directly associated with various disease conditions. Recent developments in imaging mass spectrometry (IMS) have allowed complete mapping of the phospholipid species on tissue. Phospholipid head groups carry either positive or negative charges; therefore, IMS experiments must be conducted in positive- and negative-ion mode to detect all types of phospholipids. This study was conducted to enable appropriate matrix selection and optimized matrix preparation for IMS of phospholipids in brain tissue. These IMS with optimized matrix successfully identified >100 different phospholipid species determined by both parent ion m/z and their MS/MS spectra on the same tissue.

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장소: 대구엑스코
발표코드: **PHYS2-1**
발표분야: 생물리화학의 최신 동향
발표종류: 분과기념강연, 발표일시: 금 09:00, 좌장: 이진용

Contact Mechanics of Atomic Force Microscope Tip: Molecular Simulation and Theory

장준경

부산대 나노소재공학과

Given the widespread use of atomic force microscope (AFM) in surface imaging and fabrication, we investigated the contact mechanics of AFM tips interacting with surfaces. In particular, we performed grand canonical Monte Carlo and molecular dynamics simulations for the condensation of a water meniscus between an AFM tip and a surface. In order to calculate the humidity--dependent force on the AFM tip, we developed thermodynamic integration and perturbation methods as well as a mean-field density functional theory. Our Monte Carlo calculation reproduces the typical behavior of the force-distance curve in the AFM experiment. We found the size limit for a stable meniscus is five molecular diameters. We developed a diffusion theory for the pattern grown by an AFM tip as a molecular source. We present a novel random walk model which explains both the circular and dendritic patterns found in dip pen nanolithography. Our model quantitatively reproduces the results of molecular dynamics simulation.

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발표분야: 생물리화학의 최신 동향
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 황현석

Structural and dynamical characteristics of β-amyloid fibrils revealed by two-dimensional infrared spectroscopy

김영삼

울산과학기술대 나노생명화학공학부

Recent advances in femtosecond infrared pulse generation and control permit visualization of time-dependent structure changes and fundamental physical processes in complex materials and biological systems. One of these developments is two-dimensional IR echo spectroscopy (2D IR). The possible applications of 2D IR range from liquids and aqueous solutions to proteins, large biological assemblies, and macroscopic fibrils. In this talk, I will present recent 2D IR study on structure and dynamics of β-amyloid 40 (Aβ40) fibrils. The matured fibrils formed from strands having isotopic substitution show vibrational exciton spectra having reduced dimensionality. Indeed, linear chain excitons of amide units are seen, for which the interamide vibrational coupling is measured in fibrils grown from 50% and 5% mixtures of labeled and unlabeled strands. The data prove that the 1D excitons are formed from parallel in-register sheets. The motion of water molecules close to amide groups of Aβ40 fibrils causes their vibrational frequencies to vary rapidly in time. These variations are uniquely sensed by 2D IR. It is proposed from 2D IR experiments that there are water molecules in the fibrils. The spatial locations of the water (D_2O) were inferred from the responses of 18 amide modes of Aβ40 labeled with $^{13}C=^{18}O$. Fast frequency variations were found for residues L17 and V18 and for the apposed residues L34 and V36, suggesting cavities or channels containing mobile water molecules can form between the 2 sheets. Spectroscopic analysis showed that there are 1.2 water molecules per strand in the fibrils.

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발표분야: 생물리화학의 최신 동향
발표종류: 심포지엄, 발표일시: 금 09:55, 좌장: 황현석

Biological Imaging by Broadband Coherent Anti-Stokes Raman Scattering Microsopy

성지하, *Bi-Chang Chen, *Sang-Hyun Lim

*동덕여대 응용화학과 *University of Texas at Austin, United States*

We demonstrate broadband coherent anti-Stokes Raman Scattering (CARS) microscopy and micro-spectroscopy technique based on the spectral focusing mechanism. Highly chirped broadband pump and Stokes laser create narrow vibrational excitation and generate CARS signals. Frequency switching is achieved by changing time delay between pump and Stokes laser pulse, which allows rapid and easy frequency switching. Chemical imaging and micro-spectroscopy of biological systems such as cell, mouse skin, and tissue are demonstrated for both fingerprint region (800 – 1700 cm^{-1}) and the region of CH stretching band (2800 – 3100 cm^{-1}).

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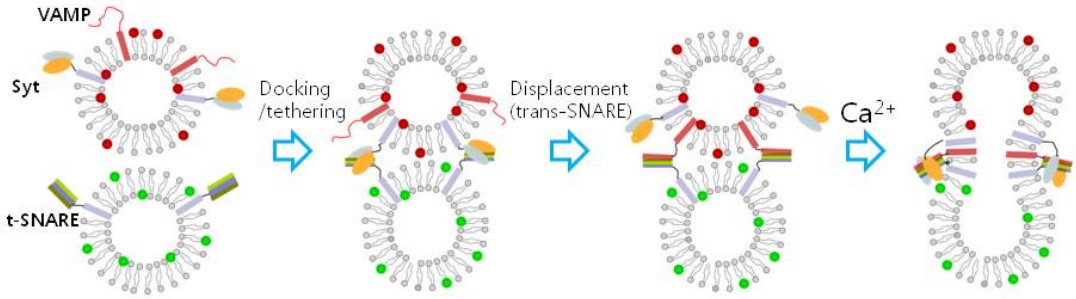
Single-Molecule and Single Cell Approach to Biological Systems

이남기, *김재열, **최봉규, ***신연균

*포항공과대 시스템생명공학부/물리학 *포항공과대 물리학과 **포항공과대 I-BIO/시스템생명공학부 ***Iowa State University*

Recent advances in single-molecule fluorescence microscope techniques have allowed single-molecule sensitivity to probe various protein-DNA interactions and their structural changes, and fundamental cellular processes in a living cell. Here I would like to introduce two single-molecule techniques: (1) a single-molecule fluorescence resonance energy transfer (FRET) technique for in vitro assay, named alternating-laser excitation (ALEX), and (2) a fluorescence microscope technique for in vivo single protein detection. ALEX is well suited for studying protein-protein interactions, protein and RNA folding, and protein-DNA interactions. Using this technique, we observed single vesicle fusion without surface-immobilization for the first time. By reducing the error due to the non-specific binding, we newly proved unknown mechanism of vesicle fusion, which plays a critical role on neurotransmitter release at the synapses of neuron. We also observed single protein in living cells by using fluorescent proteins (YFP). By detecting single or a few proteins by fluorescence, this technique allowed us to monitor the transcriptional process (the process of DNA-directed RNA biosynthesis) in living cells.

Model for membrane docking & priming



THE KOREAN CHEMICAL SOCIETY

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Controlling Neuronal Function via Silicon-Based Nanostructures

윤명한

광주과학기술원 신소재공학부

The nervous system, a three-dimensional network of interconnected neurons and glia, both maintains physiological homeostasis and enables communication with the external world by responding to stimuli, processing information, and mediating proper reactions. One of the most influential hypotheses in modern neuroscience states that the functions of these neuronal networks arise from the formation and modulation of the synaptic connections among the network's constituent neurons. To map a network's spatiotemporal connectivity and correlating it to that network's function, we need tools that can perturb and record neuronal activity in a cell-specific fashion. Toward this end, we have generated vertically-grown silicon nanowire arrays to introduce biologically important molecules into cells with minimized cytotoxicity and high delivery efficiency and, using patterned arrays, showed site-specific control of cellular functions, such as specific ion-channel knock-down and controlled glial cell proliferation. In conjunction, we have been developing planar patch-clamp arrays to monitor individual cellular activity in a mid-size neuronal network. In the future, we envision that the combination of both tools will serve as a spatially resolvable means of controlling and probing complicated neurobiological phenomena and, thus, of getting closer to cracking the neuronal communication.

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Dynamic heterogeneity and cooperativity in protein folding

정성호, *유우경, *장익수

*서울대 화학부 *부산대 물리학과*

Dynamic characterization of the folding process provides invaluable insights into the mechanism of protein folding. We propose the four-point dynamic correlation function that (i) develops a peak at the mean folding time, (ii) probes the dynamic heterogeneity via the peak width, and (iii) characterizes the strength of the cooperativity through the peak height. Here the dynamic heterogeneity refers to the multiplicity of folding pathways or the distribution of free-energy barrier heights, whereas the cooperativity to the extent of correlated residues during the folding process. We present dynamic Monte Carlo simulation results for the four-point dynamic correlation function near the folding temperature, and argue that the dynamic characteristics therefrom rationalize contrasting folding kinetics in downhilland two-state proteins, such as the non-exponential vs. exponential relaxation.

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DNA stretch approaching to full contour length in nanochannels

조규봉

서강대 화학과

Fully stretched DNA molecules are becoming a fundamental component of new systems for comprehensive genome analysis. Among a number of approaches for elongating DNA molecules, nanofluidic molecular confinement has received enormous attentions from physical and biological communities for the last several years. Here we demonstrate a well-optimized condition that a DNA molecule can stretch almost its full contour length. In addition, based on polymer physics theory, we interpret our experimental findings as a function of channel dimensions and ionic strengths. Furthermore, we develop a Monte Carlo simulation approach using a primitive model for the rigorous understandings of DNA confinement effects. Collectively, we present more complete understanding of nanochannel confined DNA stretching via the comparisons to computer simulation results and polymer physics theory.

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Azithromycin as a novel antibiotic chiral selector in chiral separation by capillary electrophoresis

박정학, *A. Praveen Kumar, 김은주, 김민지, 홍종성

*영남대 화학과 *Yeungnam University*

In capillary electrophoresis (CE), separation of enantiomers of a chiral compound can be achieved through the chiral interactions and/or complex formation between the chiral selector and enantiomeric analytes on leaving their diastereomeric forms with different stability constants and hence different mobilities. A great number of chiral selectors have been employed in CE and among them macrocyclic antibiotics exhibited excellent enantioselective properties towards a wide number of racemic compounds. The use of azithromycin (AZM) as a chiral selector has not been reported previously. This work reports the use of AZM as a chiral selector for the enantiomeric separations of seven chiral drugs and one amino acid (tryptophan) in CE. The enantioseparation is carried out using polar organic mixtures of acetonitrile (ACN), methanol (MeOH), acetic acid and triethylamine as run buffer. The influences of the chiral selector concentration, ACN/MeOH ratio, applied voltage, capillary temperature and sample solvent on chiral separation are investigated. The results show that AZM is a promising chiral selector in CE for the enantioseparation of the type of chiral drugs investigated.

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Single Molecule DNA Analysis

조규봉

서강대 화학과

Given the recent trend for using large DNA analytes for genomic applications, here we present a new DNA analysis platform for elongation and reversible immobilization of DNA molecules on the protein coated surface. Our approach is the development of a novel and simple way for presenting stretched DNA molecules reversibly immobilized on the neutravidin coated surface by changing pH and salt environments with the aid of microfluidics. On the neutravidin surface, we demonstrate restriction physical mapping on stretched T4 DNA molecules to reveal the circular permutation as a genomic application. Moreover, we demonstrate direction-controlled DNA mapping by the utilization of covalent bonds between the neutravidin surface and biotin-labeled λ DNA molecules.

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Development of a Dual-Color Fluorescence Cross-Correlation Spectrometry for Biomolecule Detection

이용일

창원대 화학과

Fluorescence correlation spectrometry (FCS) and fluorescence fluctuation spectrometry (FFS) have emerged as sensitive techniques to monitor a variety of biochemical reactions, such as protein-protein interactions, reaction kinetics, and equilibrium concentrations. An instrument for spectral cross-talk free dual-color fluorescence cross-correlation spectrometry (FCCS) which provides a readout modality for the study of enzyme activity in application areas such as high-throughput screening has been developed. Two spectrally distinct fluorophores, Cy3 and IRD800, were excited simultaneously using two different excitation sources: one poised at 532 nm and the other at 780 nm. The fluorescence information was processed on two different color channels monitored with single-photon avalanche diodes (SPADs) that could transduce events at the single-molecule level The system provided no color cross-talk (cross-excitation and/or cross-emission) and/or fluorescence resonance energy transfer (FRET), significantly improving data quality. To demonstrate the utility of the system, the enzymatic activity of APE1, which is responsible for nicking the phosphodiester backbone in DNA on the 5' side of an apurinic/apyrimidinic site, was monitored by FCCS using a double-staranded DNA substrate dual labeled with Cy3 and IRD800. Activity of APE1 was also monitored in the presence of an inhibitor (7-nitroindole-2-carboxylic acid) of the enzyme using this corss-talk-free FCCS platform.

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Practical chiral separation method development using polysaccharide-derived chiral stationary phase

Ryota Hamasaki

DAICEL Chemical Industries, LTD, Japan

For successful separation of enantiomers, various chiral stationary phases(CSPs) based on polysaccharide derivatives, cyclodexstrins, macrocyclic antibiotics, pirkle types, crown ethers, ion-exchange types and proteins have been developed. Especially, polysaccharide(cellulose and amulose) based CSPs show high chiral discrimination abilities for a wide range of racemic compounds among them[1]. They currently play an essential role in analytical and preparative separation of enantiomers. In this presentation, we will introduce polysaccharide derivatives CSPs, immobilizedor coated on a silica matrix [2], protein type CSPs, 3μm CSPs for fast and high resolution analyses that are launched recently and their applications for pharmaceutical drugs.References[1]C. Yamamoto and Y. Okamoto, Bull. Chem. Soc. Jpn., 2004, 77, 227.[2]T. Zhang, D. Nguyen and P. Franco, J.Chromatogra. A, 1191, 2008, 214-222.

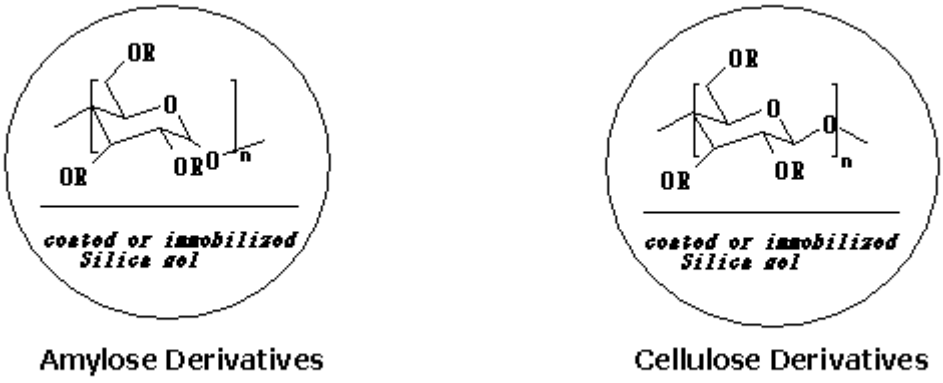

Figure 1

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Submicron silica-packed capilary electrochromatographic microchip and its applications

박종만

건국대 화학과

Microchips packed with submicron silica beads in their micro-channels are prepared. Mono-disperse colloidal silica particles were packed with high crystallinity in the micro-channels utilizing capillary action and self-assembly behavior. After cover bonding reservoirs for running buffer, sample and the waste were formed. The packing at each channel entrance was fixed with silver coating to prevent erosion of the packing structure. The silica packing at the entrances of the micro-channels served as built-in nanofilters. Reproducible electroosmotic flow control was possible without water-head problems owing to the difference between the solution levels of the reservoirs. The silica packed microchip was used for the separations of FITC-derivatives of amino acids, small sized peptides as well as metal chelates. Improvements in chip preparation and detectionsystem, effects of silica surface modification, and electrokinetic chromatographic application of the microchip will be discussed.

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Application of photothermal deflection detection technique to the analysis of aquatic nanoparticles

정의창, 조혜륜

한국원자력연구원 원자력화학연구부

Laser-induced breakdown detection (LIBD) is one of the most sensitive tools for measuring colloidal nanoparticles with diameters ranging from approximately 5-1000 nm, and concentrations ranging from parts per trillion to parts per billion. One of the established LIBD techniques is based on the acoustic detection of a shock wave generated by a laser-induced breakdown using a piezoelectric transducer. A second technology is based on the optical detection of a plasma emission using a charge-coupled device camera. In the present study, a method for determining the size of a colloidal nanoparticle by measuring the magnitude of the probe beam signal which can be remotely measured in a non-contact manner has been developed. The method using a deflected probe beam signal is intended to employ a principle by which the path of a probe beam is changed by a laser-induced shock wave, accompanying the occurrence of a laser-induced breakdown of colloidal nanoparticles. It was observed that the peak and full-width at half-maximum of a frequency distribution curve of the magnitude of a probe beam signal appear in direct correlation with the size of a nanoparticle. An application is demonstrated for measuring hexavalent uranium colloidal particles generated by the hydrolysis of free uranyl ions.

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Chemical composition and pollution characteristics of atmospheric aerosols at background area of Korea

강창희, 정덕상, 김원형, 고희정

제주대 화학과

The atmospheric aerosols have been collected at Gosan site of Jeju Island, which is one of the background sites in Korea, and the aerosol components have been analyzed to understand their chemical compositions and pollution characteristics. In the results of yearly comparison of aerosol compositions, the concentrations of NO_3^- had been increased rather smoothly compared to those of SO_4^{2-}during the study periods, indicating the change of recent energy consumption patterns in China. Meanwhile, the monthly comparison have shown that the concentrations of NO_3^- and typical soil-originated components, such as nss-Ca^{2+}, Al, Ca, Fe, Ti, Ba, etc., increased remarkably during spring season from March to May, otherwise those of nss-SO_4^{2-} were highest in June. The factor analysis verifies that the TSP aerosols in Gosan area have been estimated to be influenced largely by soil sources, followed by anthropogenic and marine sources. From the study of the concentration variations by wind direction, the concentrations of Mg^{2+}, nss-Ca^{2+}, K^+, NO_3^- and nss-SO_4^{2-} were high in westerly wind, and similarly those of Al, Fe, Ca and Ti increased in northwesterly wind. The concentration ratios of soil-originated nss-Ca^{2+}, Al, Fe, Ca, Ti, Mn, Ba and Sr between Asian Dust and Non-Asian Dust storm periods were 3.9～7.1, and the ratios of anthropogenic nss-SO_4^{2-}, NO_3^-, K^+ and S were 1.2～2.1. The backward trajectory analysis has shown that the concentrations of the anthropogenic and soil-originated components, such as nss-SO_4^{2-}, NO_3^-, NH_4^+, Pb, nss-Ca^{2+}, Al, Zn and Pb, had been increased as the air mass moved from the Chinese Continent, on the other hand, they had been decreased as the air mass moved from the Northern Pacific into Jeju area.

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Investigation of Linear and Non-linear Quantitative Structure Retention Relationship(QSRR) methods for predicting retention time in micro-HPLC

이성광

한남대 화학과

The quantitative structure-retention relationships(QSRRs) are linear or non-linear mathematical models that relate chemical structure with chromatographic retention parameter. In this study, QSRRs models were successfully developed to predict thermodynamic properties(ΔH, ΔS) of 15 polyarmatic hydrocarbons(PAH) from van't Hoff equation. Chemical structures were parameterized using PreADMET program and 1000 2D descriptors were obtained for each PAHs, including diverse structural information such as constitutional, topological, geometrical and physicochemical property. QSRR models using multiple linear regression, artificial neural net and k-nearest neighbor method is combined with genetic algorithm to select the best subsets of descriptors including cross-validation. The change of enthalpy and entropy were explained by hydrophobic and molecular size parameters, and so on. Their contributions of retention were described by standardized regression coefficient. This models also can give a virtual chromatogram of PAHs compounds in this condition.

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Cylindrical Continuous PCR Device: Real-Time PCR, Optimization-Free PCR, and On-Line Product Analysis

한종훈, 김한옥, 곽병주

포항공과대 화학과

Recently, we have developed a compact continuous-flow polymerase chain reaction (PCR) device fabricated only from solid components and demonstrated the possibility of high-throughput amplification in a segmented-flow mode. The device performs PCR by having a reaction solution flow through a long capillary wound helically around a cylindrical thermal cycler. Three thermally insulated metal heating blocks are arranged to form the cylindrical structure and run thermal cycles repetitively, in the sequence of melting, annealing, and extension. Since there is an air gap between the extension and melting blocks, the parallel, bridging parts of the capillary can be severed as windows of laser-induced fluorescence (LIF) detection for real-time PCR. The cylindrical device has been applied to optimization-free PCR by building a device with multiple cylindrical cyclers for setting different annealing temperatures. Thus it is possible to rapidly determine the optimum PCR conditions of different samples. In order to analyze the PCR products from the device on-line, a capillary gel electrophoresis microchip has been developed and interfaced with the cycler. This microchip is for sequential high-throughput analysis of different amplified DNA products and it is essentially a contamination-free method that can collect pure PCR products by isolating DNA analysis part.

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High-sensitive absorption spectroscopy using a capillary cell for the chemical speciation of actinides

조혜륜, 박경균, 정의창, 송규석

한국원자력연구원 원자력화학연구부

The chemical speciation of actinides in trace concentrations (< 10^{-6} M) is important for the determination of thermodynamic data to predict their migration behaviors in geological environment. For this purpose, several advanced techniques based on spectroscopy such as LIBD (laser-induced breakdown detection), LPAS (laser-induced photoacoustic spectroscopy), TRLFS (time-resolved laser-induced fluorescence spectroscopy) have been applied. In this paper, an absorption spectroscopic technique using a capillary cell with the optical path length of 100 cm was applied for qualitative and quantitative analysis of actinides' species. The limits of detection for the most actinides' species were below micro molar concentrations. As an application, the absorption features of Pu(VI)-OH species in micro molar concentrations were investigated. The formation constants of Pu(VI)-OH species were precisely determined with considering trace amounts of Pu(V) species.

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Structural Characterization of Small Biomolecules Using Ion Mobility Spectrometric Techniques

김준곤

포항공과대 화학과

We present an augmentation to the experimental and theoretical study of structural characterization of small biomolecules using electrospray ionization ion mobility spectrometry in N2 drift gas. Amino acids, ammonium cations, and phosphatidylcholines (PC) are studied in positive ion mode and carboxylic acids are investigated in negative ion mode. We further present the investigation of an experimentally observed correlation between mass of biomolecules and gas phase mobilities by computational modeling. A modified trajectory method for the ion-neutral interaction, to account for the potential associated with the non-spherical drift gas N2, has been applied to predict cross sections of polyatomic biomolecule ions and to test the sensitivity of collision cross section to details of the ion-neutral interaction. In addition, the investigation of field effect to the ion's gas phase energetic and ion mobility constant will be discussed with an example of observed correlation between mass and mobility of saturated PC and deviation of the unsaturated PC cation from the correlation line.

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Identification of benzalkonium chloride from stainless steel MALDI plates

김정권

충남대 화학과

Peaks originating from unknown compounds on stainless steel plates used in matrix-assisted laser desorption/ionization (MALDI) mass spectrometers are observed around m/z 304.3, 332.3, 360.4, and 388.4 regardless of the matrix and/or solvent and are even observed with bare plates. These peaks were characterized using three different types of MALDI-MS instrumentation: MALDI-TOF MS, MALDI-TOF/TOF MS, and MALDI-FTMS. The fragmentation data from MALDI-TOF/TOF MS and accurate mass determination by MALDI-FTMS enabled identification of the chemical formulae and structures. The unknown compounds are, in fact, likely benzylalkylmethylammonium salts, as confirmed by closely matching fragmentation patterns with a commercially available benzalkonium chloride.

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Development of LC/MS-based reference methods for food analysis

김병주, 안성희, 이준희

한국표준과학연구원 삶의질측정표준본부

Food safety issues are attracting considerable public attentions and prompts regulatory actions due to recent incidents related unsafe food such as dairy products contaminated with melamine. As food trading across national boards is growing worldwide, reliable food testing becomes one of the important tools for safeguard against contaminated or adulterated food and for ensuring the quality of food. Our laboratory is developing reference methods for food analysis which can provide national standards to ensure reliability of food testing laboratories. Those reference methods are based on Isotope Dilution Mass Spectrometry (IDMS) in connection with chromatographic techniques such as GC and LC because IDMS is known to provide accurate analytical results without systematic bias through the accurate correction of the recovery on target analytes along the sample clean up processes. Presented are our recent results on the development of IDMS method based on LC/MS for the analysis of food contaminants such as antibiotics, food additives, and pesticides residues and nutrients (which is monitored to control quality of food).

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발표코드: **ANAL2-5**
발표분야: 최근의 분석화학 분야 연구현황
발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 김정권

Bioelectronic Nose based on Membrane-Carbon Nanotube Hybrid Structures

김태현

순천향대 화학과

Proteins in cell membrane have been drawing attention due to their versatile functionalities such as ion transfer for neuronal activity and selective binding for sensory systems. However, it is still very di±cult to manipulate and study those proteins because they easily lose their functionalities without lipid membranes. We developed a method to coat lipid membranes containing various functional membrane proteins on single-walled carbon nanotube (swCNT)-based field efect transistors (FETs). In this hybrid structure, the activity of membrane proteins can be monitored by underlying swCNT-FETs, allowing us to easily study the functionalities of membrane proteins. Furthermore, we built advanced devices based on these hybrid structures. For an example, we coated lipid membrane containing `olfactory receptors' on swCNT-FETs, resulting in `bioelectric nose' systems. The bioelectric nose system had high sensitivity and human nose-like selectivity to odorant molecules. This talk will also discuss about the future prospect of these membrane-CNT hybrid structure.

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Development of Amperometric S-Nitrosothiol Sensors by Using Organometallic Catalysts

차완식, *Sangyeul Hwang, *Mark E. Meyerhoff

*한국원자력연구소 원자력화학연구부 *University of Michigan*

S-Nitrosothiols (RSNOs), such as S-nitrosoglutathione, S-nitrosocysteine, S-nitrosoalbumin (AlbSNO) and S-nitrosohemoglobin (HbSNO) exist in fresh blood and are thought to serve as stable carriers of transient NO in the bloodstream. Total RSNO levels in blood may serve as an indicator of NO production by the EC, and also may control endogenous platelet function. Hence, measurement of RSNO levels could be useful as a prognostic tool to assess the risk of thrombotic events (e.g., heart attacks, strokes, etc.) for patients, and to detect the onset of systemic sepsis and associated septic shock, in which high levels of NO are produced from activated macrophages. Recently, novel types of amperometric RSNO sensors have been developed to directly detect RSNO species in biological samples, e.g., whole blood. A highly sensitive NO sensor reported earlier has been modified with catalytic layers capable of decomposing RSNO and producing NO directly at the surface of the sensing tip. Amperometric current resulting from NO oxidation on the working electrode varies proportional to the RSNO levels in a sample solution. Various catalysts including Cu(II), organoselenium (RSe), and organotellurium (RTe) catalytic species as well as glutathione peroxidase (a selenoenzyme) have been immobilized to form a catalytic layer at the surface of the amperometric NO probes. Recently, it is shown that RSNO sensors based on RSe-DM exhibit lower detection limit (20 nM ~ 10 μM) and higher sensitivity, and also enable macromolecular RSNO quantification via transnitrosation with low-molecular-weight thiols (including detection of AlbSNO and HbSNO). In this presentation, response characteristics observed during RSNO detection will be compared and discussed based on the nature of catalytic sites and their RSNO decomposition mechanisms proposed.

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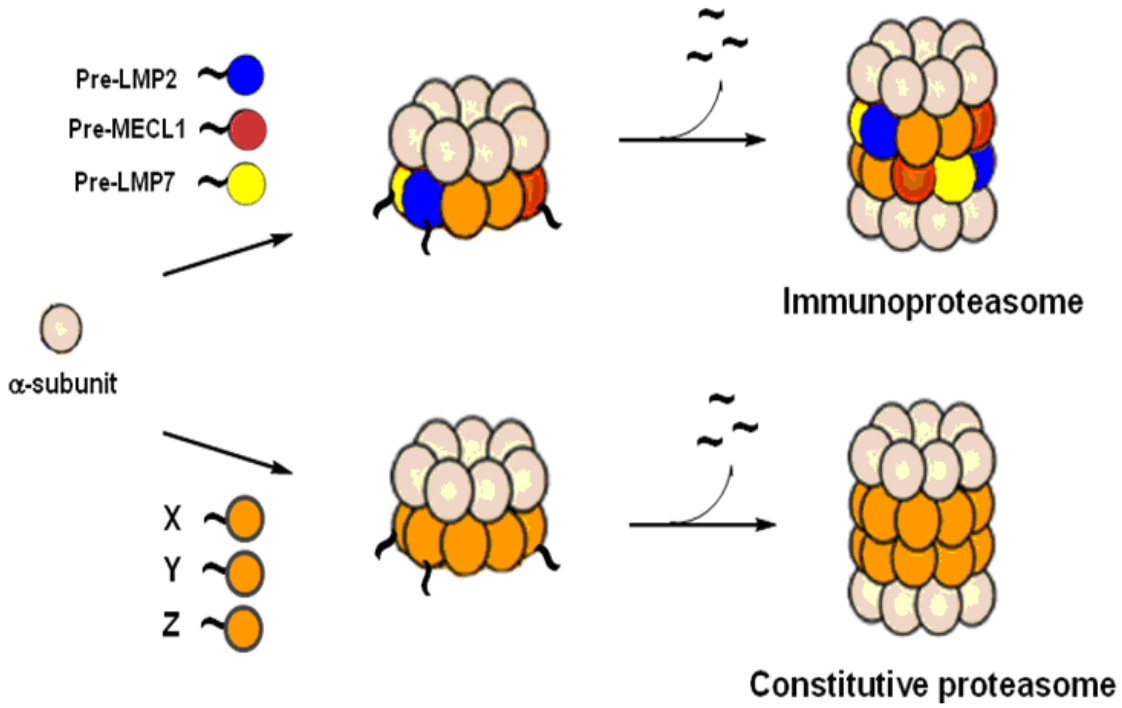
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이연

Chemical Genetics: Probing Proteasome Biology with Small Molecules

Kyung-Bo Kim

University of Kentucky, U.S.A.

The multiprotease complex proteasome, which is present in all eukaryotic cells, is responsible for degradation of the majority of cellular proteins involved in many important cellular processes, such as cell cycle progression, development and inflammatory responses. The FDA approval of bortezomib, a first-in-class general proteasome inhibitor drug, for the treatment of refractory multiple myeloma has validated the proteasome as a clinical target for cancer treatment. However, the toxicity of this broadly acting proteasome inhibitor to non-tumor cells is a major clinical concern. The immunoproteasome, an alternative form of the constitutive proteasome, has recently gained much attention as an alternative target. However, the immunoproteasome remains largely untapped for drug discovery and the biology of the immunoproteasome is poorly understood. In this talk, I'll describe our efforts to unravel complex and untouched world of the immunoproteasome. Specifically, my talk is directed towards target validation and functional studies of the immunoproteasome in cancer using a variety of chemical probes. Development of novel probes that provide high temporal and spatial control of protein functions has become critical in the investigation of complex biological processes in vitro and in vivo. While classical manipulation of protein expression levels at the DNA or RNA levels has provided a powerful tool to study protein function, their widespread applications are somewhat limited by the lack of temporal and spatial control. In this talk, I'll show a novel class of probes that target protein for ubiquitination and subsequent degradation by the proteasome.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
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유전자 및 단백질 합성 기술의 개발과 응용

방두희

연세대 화학과

유전자와 단백질 합성기술은 이미 생명, 의•과학, 에너지 산업 등의 다양한 분야에 적용되고 있다. 합성 유전자를 이용한 예는, 최적화된 코돈 유전자를 이용한 항체 약의 합성, 변형된 바이러스 게놈 합성을 통한 백신의 개발, 디자인-합성된 genetic pathway 를 이용한 가치 있는 약 분자 생산, 그리고 합성 게놈으로 만들어진 세포를 통한 바이오 연료의 생산 등으로 매우 다양하다. 본 세미나는 우리가 개발해 온 유전자와 단백질 합성 기술을 논의한다. 또한 DNA 마이크로 칩을 이용하여 빠른 속도로 유전자를 합성하기 위한 최근 연구 경과를 논의한다.

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Targeted Genome Rearrangements in Higher Eukaryotic Cells Using Engineered Zinc Finger Nucleases

김진수

서울대 화학부

We present a novel approach for targeted rearrangements of genomic segments in human and other eukaryotic cells using engineered zinc finger nucleases (ZFNs). ZFNs are artificial restriction enzymes made by fusing tailor-made DNA-binding zinc finger arrays to the FokI nuclease domain. ZFNs induce site-specific DSBs in the genome, whose repair via HR or NHEJ gives rise to targeted mutagenesis, and, thus, are powerful tools for genome engineering in various cell lines and organisms. We found that ZFNs designed to target two different sites in a human chromosome could introduce two concurrent DSBs in the chromosome and gave rise to targeted deletions of the genomic segment between the two sites. Using this method, we were able to delete pre-determined genomic DNA segments in the range of several hundred base pair (bp) to 15 mega bp in human cells at frequencies of 10-3 to 10-1. These high frequencies allowed us to isolate clonal populations of cells in which the target chromosomal segments were deleted by screening individual cells separately expanded in a 96-well plate. Many of the DNA sequences of deletion junctions showed small insertions or deletions and microhomologies, indicative of DNA repair via NHEJ. Unlike other genome engineering approaches employing recombinases and meganucleases, ZFNs do not require pre-insertion of target sites into the genome and allows precise manipulation of endogenous genomic scripts in animal and plant cells. Thus ZFNs would be broadly useful as tools in reverse genetics, biotechnology and gene therapy.

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A reversible internal light switch for living biological systems from dye-crosslinked dendritic nanoclusters

김윤경

한국생명공학연구원 바이오나노연구센터

Photochromic compounds typically show a reversible conformational change (e.g., cis-trans isomers, ring-closed and ring-open forms) upon alternate irradiation with UV and visible light. Accordingly, photochromic compounds originally captured attention among scientists for their potential use in optical storage media. Only a limited number of photochromic systems have appeared to date relevant to biological applications. For instance, photochromic dyes have been incorporated into biological systems for high contrast imaging applications or to regulate biological functions through the photocontrolled conformational switching. Here, a novel dendritic nanostructure was constructed by oligomerizing the dendrimer with a bifunctional diarylethene derivative (one of the most efficient photochromic scaffolds) as a crosslinker. This photochromic dendritic system was further derivatized with a highly fluorescent sulfoindocyanine dye of the matching FRET wavelength for the fluorescence photoswitching by photochromic FRET. By appropriately modifying the surface, these dendritic nanoclusters became relatively nontoxic and were readily taken up by cells for photoswithcing inside the living systems. Furthermore, here we disclose, for the first time, the application of photochromic systems to living vertebrates as a reversible internal light switch.

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발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 김윤경

Fabrication of Paramagnetic Nanoparticles as a Contrast Agent for Magnetic Resonance Imaging

이인수

경희대 응용화학과

Nano-sized colloidal particles have many superior properties when used as MRI contrast agents and thus have the potential to allow for the specific and sensitive visualization of targets at low concentration. The further development of nanoparticulate MRI contrast agents will require materials that have much more enhanced relaxivity and can operate at much lower concentrations of potentially toxic metal ions. In this context, hollow nanoparticles with interior void spaces are attractive candidates for advanced MRI contrast agents owing to their large water-accessible surface area, which is able to carry high payloads of MR-active magnetic centers. In this study, hollow manganese oxide nanoparticles were synthesized by selectively carving away the core from nanoparticle having MnO core coated by Mn3O4 shell. The hollow nanoparticles showed the greatly enhanced relaxivities, comparing with those having solid interior. Their efficient cellular uptake allowing for the delivery of anticancer reagents was also examined, demonstrating their potential as bifunctional medical system combining diagnostic imaging and drug treatment. In this presentation, we also report an approach for fabricating gadolinium based paramagnetic contrast agent from layered gadolinium hydroxide (LGdH) compound. A novel method for modifying the surface of MR contrasting LGdH layers was developed to provide them with water- and bio-compatibility and acid-resistance, which are essential for medical applications. The exfoliated LGdH layers surface-modified by newly developed method displayed the potential utility as a multimodal probe combining MR and fluorescence imaging.

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Selective gene delivery for cancer therapy using nanoparticles

김근식, 김동은

건국대 생명공학과

Targeted gene delivery is essential if cancer treatment is to become a reality with this form of therapy. For the past few decades, there has been a considerable research interest in the area of drug or gene delivery using particular delivery systems as carriers for small and large molecules. Particular systems like nanoparticles have been used as a physical approach to improve the delivery properties of various types of drug molecules or genes. They have been used in vivo to protect the drug or gene entity in the systemic circulation. Various polymers or cationic liposomes have been used in the formulation of nanoparticles for gene delivery research to increase therapeutic benefit, while minimizing side effects. In this talk, various aspects of nanoparticles formulation, characterization, effect of their characteristics and their applications in delivery therapeutic genes will be presented. Especially, this talk will focus on the following three issues; anti-TAG-72 immunoliposome using a humanized anti-TAG-72 antibody for targeting colon cancer, bifunctional dendrimer using galactose for targeting hepatocyte, and aptamer conjugated-liposome (Aptamosome) using PSMA-specific aptamer for targeting PSMA on prostate cancer. These results demonstrate the enhancement of specific gene transfer by the modification of nanoparticles in the design of new therapeutic strategies for cancer.

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Bioreducible polymeric gene delivery carriers with cell penetrating functionality

Tae-il Kim

University of Utah, U.S.A.

Bioreducible polymers, which contain characteristic disulfide linkages, can be degraded in response to redox potential through thiol-disulfide exchange reaction. So, bioreducible polymeric gene delivery carriers can acquire benefits such as decreased cytotoxicity and controlled release of genetic materials due to the biodegradation in cells, maintaining the stability in aqueous solution, unlike other hydrolytic polymers because cytoplasm contains 0.5-10 mM of glutathione, most abundant intracellular reducing molecule, keeping highly reductive environment inside cells. Arginine or guanidine is also reported to play a leading role for cell penetration of cell penetrating peptides. Therefore, introduction of arginine or guanidine to bioreducible polymer was tried to combine the structural advantages of bioreducibility and cell penetrating functionality for efficient gene delivery systems. Arginine-grafted or guanidinylated bioreducible polymer (ABP or GBP) formed polyplexes with pDNA, releasing pDNA through degradation under reductive condition. Their cytotoxicity was minimal and superior transfection efficiency of the polymers to PEI25k was observed, although cellular uptake assay didn't display significant differences between them. Confocal microscopy observation for intracellular trafficking of the polyplexes suggested that GBP possesses strong nuclear localization ability for pDNA delivery which can lead to high transfection, explaining the discordance. Therefore, it is concluded bioreducible polymers with cell penetrating functionality can be safe and potent gene delivery carriers

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발표분야: 핵산생화학과 생명과학에의 적용
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 김동은

RNA nanostructures for therapeutic applications

이동기

성균관대 화학과

Chemically synthesized small interfering RNAs (siRNAs) can mediate efficient gene silencing in a sequence-specific manner by utilizing the endogenous RNA interference (RNAi) pathway. However, the current standard synthetic siRNA structure, which harbors a 19–base pair duplex region with 3' overhangs of 2 nucleotides (the so-called 19+2 form), exhibits sequence-independent non-specific effects and poor cellular delivery by cationic polymers, which posed challenges to the gene silencing in research and development of RNAi therapeutics. Here we introduce novel siRNA structural variations that can significantly benefit the siRNA-mediated gene silencing. First, we present truncated siRNA backbone structures with duplex regions shorter than 19 bp (referred to as asymmetric shorter-duplex siRNAs or asiRNAs) that can efficiently trigger gene silencing without non-specific effects triggered by conventional 19+2 siRNA scaffold, such as sense strand-mediated off-target gene silencing and saturation of the cellular RNAi machinery. We also show multi-armed gene silencing RNA structures called tsiRNAs, which not only mediate multiple gene silencing, but also show enhanced cellular delivery by cationic polymers such as polyethyleneimine (PEI). These novel siRNA structural variants exemplify the structural flexibility of gene silencing RNAs, and have the potential to become important alternatives to the current siRNA structure for functional genomics and therapeutic applications.

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NMR spectroscopic elucidation of the B-Z transition of a DNA duplex induced by the Z-DNA binding proteins

이준화

경상대 화학과

Left-handed Z-DNA is in a higher energy conformation than right-handed B-DNA and forms in a polymer of alternating pyrimidine-purine nucleotides. The Z-DNA binding domains of human ADAR1 (hZa_{ADAR1}), yatapoxvirus E3L ($yabZa_{E3L}$), and human DAI (hZb_{DAI}) preferentially bind Z-DNA rather than B-DNA with high binding affinities. The co-crystal structures of these Z-DNA binding proteins complexed to Z-DNA showed that one monomeric Z-DNA binding protein binds to one strand of double-stranded DNA and a second monomer binds to the opposite strand with 2-fold symmetry with respect to DNA helical axis. In order to characterize the molecular recognition of Z-DNA by Z-DNA binding proteins, we performed CD and NMR experiments with complexes of hZa_{ADAR1}, $yabZa_{E3L}$, and hZb_{DAI} bound to d(CGCGCG)2 (referred to as CG6) produced at a variety of protein-to-DNA molar ratios. This study suggests an active B-Z transition mechanism in which the hZa_{ADAR1} protein first binds to B-DNA and then converts it to left-handed Z-DNA, a conformation that is then stabilized by the additional binding of a second hZa_{ADAR1} molecule. In order to investigate the sequence effect on the DNA binding affinity and B-Z conversion activity of the hZa_{ADAR1}, we also performed NMR experiments on complexes between the hZa_{ADAR1} and non-CG-repeat DNA duplexes, d(CACGTG)2 or d(CGTACG)2, with a variety of protein-DNA molar ratios. During the B-Z transition, hZa_{ADAR1} exhibits the sequence preference of d(CGCGCG)2 >> d(CACGTG)2 > d(CGTACG)2 through multiple sequence discrimination steps. These results can explain how hZa_{ADAR1} selectively recognizes the alternating d(CG)n sequence in a long genomic DNA.

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Chemistry, properties and applications of PNA (Peptide Nucleic Acid)

김성기

(주)파나진

Peptide Nucleic Acid (PNA) is nucleic acid analog in which the sugar phosphate backbone of natural nucleic acid is replaced with a N-(2-amino-ethyl)-glycine unit, resulting in an achiral and uncharged mimic. It was firstly reported 18 years ago and has received great attention due to its several favorable properties including chemical and thermal stability, resistance to the nuclease and protease, stronger and faster binding affinity to the complementary nucleic acid, hybridization under low salt concentration, and higher specificity and sensitivity to the single mismatch. Specially, PNA has attracted major attention at the interface chemistry and biology because of its interesting chemical, physical, and biological properties and potential to act as an active component for diagnostics, biological, and pharmaceutical applications.In this seminar, I will introduce a novel synthetic method of PNA oligomer, the superiority of PNA chip to DNA chip, and point mutation detection technology using PNA for diagnostics, which are developed at Panagene.

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발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 김동은

Modified Nucleic Acid Systems for Biomedical Applications

김병현

포항공과대 화학과

Nucleic acids have been emerged from various research areas such as DNA computing, nano-size structures using DNA, sensors recognizing mRNA and DNA, oligonucleotide therapeutics, and others. There are a lot of interests in nucleic acid as a fundamental molecule for chemist to study and use as an object for chemical building blocks. Chemical modification of nucleic acid systems plays an important role to obtain more effective and stable materials.From nucleoside to oligonucleotide, chemical modification is open to any part of nucleic acid. We have focused on the synthesis of new phosphoramidites to incorporate into the oligonucleotides and have constructed our modified nucleic acid systems for biomedical applications.In this symposium, we would like to discuss our research efforts towards oligonucleotides functionalized with steroidal derivatives and cationic amine moieties to enhance their cell permeability. We all also talk about our syntheses of modified oligonucleotides containing fluorescent tags for use as molecular probes (molecular beacons) to detect single-nucleotide polymorphisim (SNP) in nucleic acids, and to monitor secondary structure of various nucleic acids such as B-Z transition, G-quadruplex structures, and i-motif structures.

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Structural basis for DNA recognition by DAI, a cytoplamic DNA sensor of the innate immune response

김경규

성균관대 의학과

Z-DNA is stabilized by the interaction with Z-DNA binding proteins which contains one or two Z-DNA binding domains (ZBDs). Among them, DAI takes a role in the DNA-mediated innate immune response. The second ZBD of human DAI (hZ′ DAI) shows significant sequence variations from other known ZBDs. The crystal structure of hZ′ DAI/Z-DNA complex reveals that hZ′ DAI has a similar fold to other ZBDs, but adopts a distinct DNA binding mode. It is thought that the two ZBDs of DAI bind together to DNA and are both necessary for full B-to-Z conversion. It is possible that binding of two DAIs to a DNA duplex brings about dimerization of DAI that is necessary for facilitating DAI-mediated innate immune activation.

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DNA-Carbohydrate Conjugate & the Application to Glycobiology

김태우

경희대 동서의학대학원

DNA 는 생물학적 활성을 가진 리간드의 배열(숫자, 간격)을 수십나노 이하에서 조절할 수 있는 nano-scaffold 이다. 이런 DNA 의 특성은 기존의 합성 혹은 고분자 scaffold 와 차별화되며, multivalent interaction 특히 세포간 커뮤니케이션에 관여하는 Glycan cluster 와 GBP (Glycan Binding Protein)의 상호작용 연구에 이상적인 scaffold 로서의 DNA 응용에 우리를 주목하게 한다.이런 응용을 위해서는 glycan 를 DNA 에 연결하는 합성적 방법의 개발이 전제되어야 한다. 이를 위해 Hydroxylamino 유도체를 합성하였고, 이 분자의 Chemo- and Stereoselective glycan 환원 말단 수식을 C1' 13C labeled Glucose, N-Ac Galactose 를 통해 확인하고 최적화하였다. Hydroxylamino 유도체를 통해 당에 N3 (azide) 작용기를 도입하였고, ethynylated DNA 와 해당 당을 CuAAC (Cu-Catalyzed Azide-Alkyne Cycloaddition)를 이용하여 공유결합으로 연결하는 합성 방법을 개발하였다.

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발표분야: 분자인식화학 국제심포지엄
발표종류: 분과기념강연, 발표일시: 목 13:20, 좌장: 서홍석

Discovery of Novel Therapeutic Agents using Molecular Diversity and Chemical Biology

박승범

서울대 화학부

Diversity-oriented synthesis (DOS), which aims to populate the chemical space with skeletally and stereochemically diverse small molecules with high appending potentials, has been proven to be an essential tool for the discovery of bioactive small molecules. The incorporation of privileged substructural motifs became an essential element in DOS pathways. Multistep, practical solid-phase strategies for the synthesis of benzopyran-embedded polyheterocycles and natural product-like diaza-bridged heterocycles have been developed. These synthetic pathways were established through the divergent approach from unique key intermediates. In addition, we constructed various drug-like small molecule library containing novel molecular frameworks embedded with privileged substructures such as benzodiazepine, pyrazole, pyrazolopyrimidine, and pyrimidine. The each key step was regioselective and diastereoselective to provide final products as single diastereomers in exceptional yields and purities without further purification, which was confirmed by NMR structural study and LC/MS analysis.In this presentation, I would like to share the current approach for the discovery of novel therapeutic agents using molecular diversity constructed by our DOS exercise along with chemical biology approach. The various high throughput screening revealed the biological activities of synthetic small molecules along with their potential applications as new therapeutic agents. We also confirmed their biological activities in animal models. Finally, I would like to introduce our effort on the target validation using PACID technology with 2D gel electrophoresis.

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발표분야: 분자인식화학 국제심포지엄
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이창희

Design, Synthesis, and Applications of Bioinspired Nanoscale Adhesive Agents

Steven C. Zimmerman

University of Illinois, USA

The high fidelity of DNA replication is partly due to base-pairing specificity. Inspired by DNA we have developed a series of artificial base-pairs that form hydrogen-bonded complexes that exhibit significantly higher stability and higher fidelity relative to their natural counterparts. Particularly useful is a urea of guanosine (UG unit) which pairs with 2,7-diamidonaphthyridine (DAN unit). These units can be readily incorporated into small molecules and macromolecules, and attached to nanoparticles and surfaces, in some cases using "click chemistry." This talk will describe these nanoscale adhesion promoters and the broad range of supramolecular structures that can be produced. The physical organic approach to optimizing their performance will be one theme. Applications possible with these very high affinity recognition units will be highlighted. The agents have been particularly useful in enhancing the energetics at normally unfavorable interfaces at the molecular and materials level. Additionally, stimuli responsive recognition units will be introduced as a way to turn the recognition on and off. The ability to orthogonally address recognition events at the molecular level provides a degree of control necessary to replicate the biocomplexity of naturally occurring systems.

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발표분야: 분자인식화학 국제심포지엄
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 이창희

Synthesis and Self-Assembly Properties of Conjugated Block Copolymers

Christopher W. Bielawski

The University of Texas at Austin, U.S.A.

The self-assembly of conjugated block copolymers has emerged as a promising approach to achieving the hierarchical and morphological control needed for understanding and optimizing the charge separation and shuttling processes inherent to organic photovoltaic (OPV) devices. We will describe our latest efforts toward synthesizing various polythiophene-containing rod-rod and rod-coil diblock copolymers, particularly those that are capable of self-assembling into higher order structures. In particular, we will present two complementary synthetic approaches developed in our laboratories: a grafting-from approach, where an end-functionalized polythiophene is used as a macroinitiator for the chain extension polymerization of a second block, and grafting-to approach, whereby the constituent homopolymers are independently synthesized and then subsequently linked together. The copolymers prepared using these methods containg homopolymer blocks that were designed to assemble into micelles, wormlike micelles, and other higher order structures in solution, and adopt similar advanced structures in the solid state. Characterization of these materials will be discussed, as well as their potential applications in organic photovoltaics and other electronic devices.

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발표분야: 분자인식화학 국제심포지엄
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이창희

Development of sensing technology using novel host molecules

김종승

고려대 화학과

A novel coumarin-based fluorogenic probe bearing the 2-picolyl unit was developed as a fluorescent chemosensor with high selectivity and suitable affinity in biological system toward Cu2+ over other cations tested. The fluorescence on-off mechanism was studied by femtosecond time-resolved fluorescence (TRF) upconversion technique and ab initio calculations. The receptor can be applied to the monitoring of Cu2+ ion in aqueous solution with a pH span 4-10. To confirm the suitability of the ligand for biological applications, we also employed it for the fluorescence detection of the changes of intracellular Cu2+ in cultured cells. The results indicate that the ligand should be useful for the fluorescence microscopic imaging and the study on the biological functions of Cu2+.A new chemosensor-based approach to the detection of nitrated aromatics is described. It involves the analyte-induced quenching of excimer emission of a dipyrenyl calix[4]-arene (L). In the solid state, the complex L•TNT consists of a supramolecular crystalline polymeric structure, whose formation appears driven by intermolecular π-π interactions between two pyrene units and a TNT molecule held at a distance of 3.2 ~ 3.6 Å, as well as by intra- and intermolecular H-bonds among the amide linkages.

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발표분야: 분자인식화학 국제심포지엄
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 윤주영

Chaos vs. Control: The Chemistry of Large Molecular Systems in Water

Brent L. Iverson

The University of Texas at Austin, U.S.A.

Several projects will be described that span the interface of chemistry and biology. On the synthetic chemistry side, our work revolves around the use of complementary aromatic donor-acceptor interactions in aqueous solution to control folding and assembly of complex molecular systems. Complementary aromatic donor-acceptor stacking units offer the advantages of a strong hydrophobic effect driving force in water combined with recognition sufficient to organize flexible molecular systems. Recent work has centered on amphiphilic folding molecules that undergo an irreversible conformational change to enable the creation of the first abiotic highly ordered aggregate reminiscent of amyloid formation, a process that is indicated in a growing number of neurodegenerative diseases, most notably Alzheimer's disease. In addition, we continue to develop a series of molecules that bind to specific sites on double-stranded DNA through a novel mode of interaction referred to as threading polyintercalation. On the molecular biology front we have developed several technologies that enable us to engineer desirable properties into proteins of practical interest, including antibodies and enzymes intended for use as therapies. For example, we have engineered an antibody that can prevent and cure anthrax. Most recently, we have been engineering enzymes such as proteases (enzymes that cleave other proteins) in an effort to create catalytic therapies to treat cancer or inflammatory disease.

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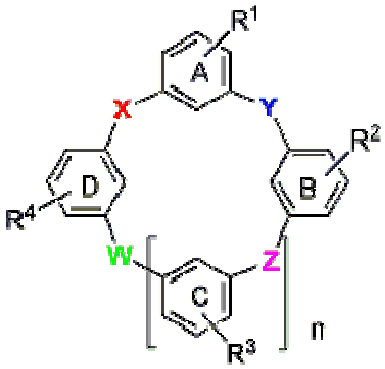
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 윤주영

Supramolecular Chemistry of Functional Heteracalixaromatics

Mei-Xiang Wang

Tsinghua University, China

The sophistication of the design and synthesis of novel and functional macrocyclic host molecules has always been one driving force to promote the major advances in supramolecular chemistry. In recent years, we have been investigating the supramolecular chemistry of heteroatom-bridged calixaromatics or heteracalixaromatics. In comparison with conventional calixarenes, introduction of oxygen and nitrogen atoms as the bridge linkages in calix(hetero)aromatics has resulted in a wide variety of fine bridge-tuned macrocyclic cavities because oxygen and, particularly, nitrogen atoms can adopt sp^3 and sp2 hybrid configurations to form different degree of conjugation with the neighboring (hetero)aromatics. In this presentation, I will discuss the syntheses, structures, functionalizations and molecular recognitions of diverse heteracalixaromatics (Figure 1).



X, Y, Z, W = heteroatoms
A, B, C, D = (hetero)aromatics

Figure 1. Structure of heteracalixaromatics

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발표종류: 심포지엄, 발표일시: 목 17:30, 좌장: 윤주영

Macrocyclic Oligopyrroles as Versatile Molecular Receptors and Chemosensors

이창희

강원대 화학과

Development of molecular receptors possessing high affinity and selectivity for various targeted guest molecules, have been an ongoing challenge in the field of supramolecular chemistry. As results, many model systems utilizing various molecular scaffolds have been developed and studied. Among them, calix[4]pyrroles have been shown to bind anions in organic or aqueous organic media and the isolation of the binding domain from matrix enhances the anion binding affinity of calix[4]pyrroles. Based on these our previous results, we have designed and synthesized various calix[4]pyrrole-based ion/molecular receptors. The calix[4]pyrrole bearing diametrical strap on one side of the molecule showed many interesting binding characteristics depending on the strapping elements. For example, the oligoethers strapped system exhibited anion-modulated, cation selective binding. When pyrrole units were replaced with other aromatic systems, the molecules displayed neutral molecule recognition such as fullerene and TNT. The systematic binding studies indicated that the modified systems are better receptors for anions, ion-pairs and neutral molecules. When the hybrid systems contain chromogenic or fluorogenic reporter groups, the system became excellent chromogenic or fluorogenic chemosensors. The dicyanovinyl-substituted calix[4]pyrroles can be selective ratiometric chemosensors for cyanide anion. The versatility of the calixpyrrole-based chemosensor systems will be presented.

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발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 13:20, 좌장: 이희윤

Development of ammonium dinitramide (ADN) at FOI

Patrick Goede, Niklas Wingborg, Nikolaj Latypov

FOI, Swedish Defence Research Agency, Sweden

ADN is an interesting new oxidizer which has a potential both to increase the performance of solid rocket propellants and to reduce the signature. Further on ADN has shown great potential as a primary component in high perfomance underwater explosives. FOI has studied ADN since the mid 90:s and has since then studied many aspects of the molecules and its applications. This includes synthesis, scale-up, analyses, stability, particles, formulation, sensitivity and other properties of both the raw material and prepared propellants and high explosives. This presentation will give a review of mainly the chemical aspects of the work done at FOI and will also discuss the future of our research in this area.

THE KOREAN CHEMICAL SOCIETY

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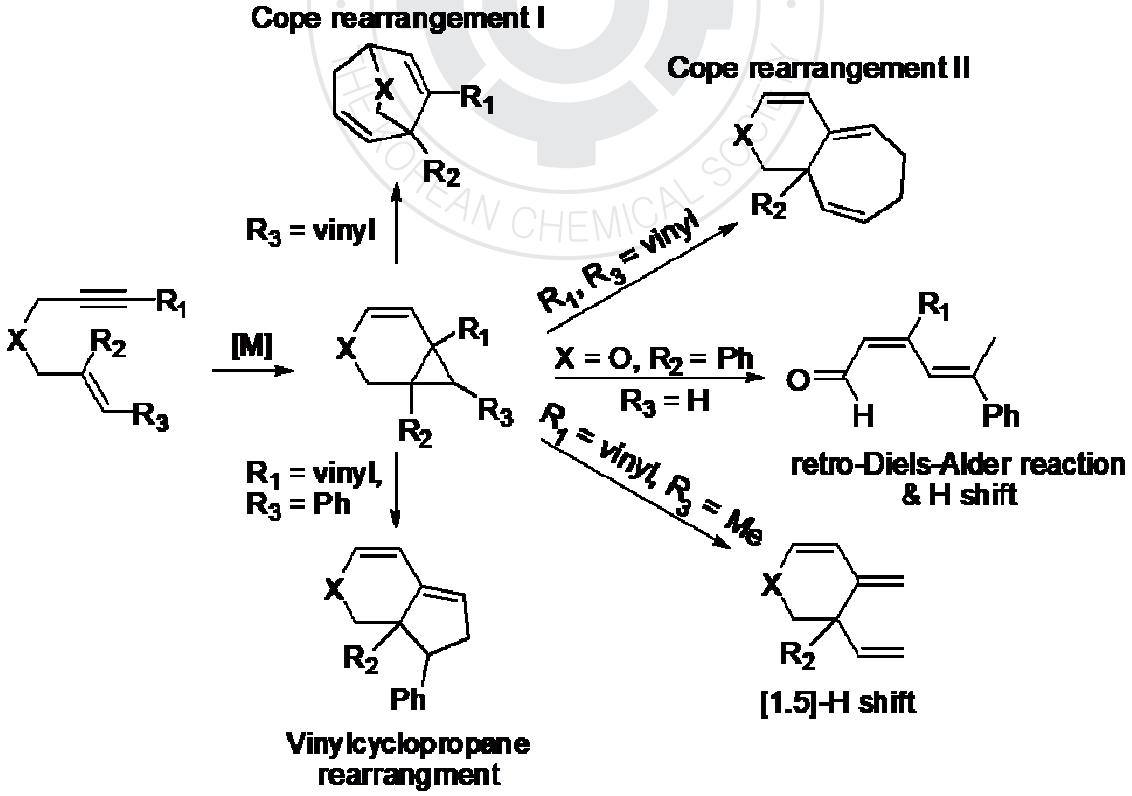
발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 장석복

Platunum and Rhodium-Catalyzed Cycloisomerization

정영근

서울대 화학부

본 발표에서는 백금 및 로듐 촉매를 이용한 고리이성질화 반응에 의한 cyclopropanated 화합물의 합성과 이렇게 해서 생성된 cyclopropanated 화합물의 백금 촉매에 의한 thermal rearrangement 를 이용한 다양한 화합물의 합성에 대해서 논의하고자 한다.



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장소: 대구엑스코
발표코드: **ORGN/INOR-3**
발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 장석복

Gold(I)-catalyzed reactions : A flexibility-driven approach

이영호

포항공과대 화학과

One of the main goals in developing new catalytic reactions is to maximize the molecular diversity in a highly controlled manner. Gold complexes are becoming a very powerful tool for this purpose. mostly because of their unique reactivity towards alkynes. In this presentation, our recent development in this area will be disclosed. Also, the issue of chemo- and stereoselectivity will be discussed.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 장석복

Novel Zirconium Complexes Containing Bidentate Benzotriazole Ligand

이준승

전남대 화학과

Treatment of CpZrCl3 with 1 equiv of 2-(2H-benzo[d][1,2,3]triazol-2-yl)-4,6-di-tert-pentylphenol (LigH) in THF or toluene afford monomeric 1 or dimeric 2, respectively. THF could transform dimeric 2 with two bridging chlorides into monomeric 1 within few minutes at room temperature. The reaction between LigH and 2 equiv of CpZrCl3 gave novel dimeric complex 3 linked by three bridging chlorides. The monomeric complex 4 containing two deprotonated LigH and two Cl ligands could be obtained by the reaction between 2 equiv of LigH and Zr(NMe2)¬4 in toluene and subsequent addition of Me3SiCl. The molecular structures of 1 – 4 were determined by single crystal X-ray crystallographic method. In the presence of methylalumoxane (MAO) as a cocatalyst, the precursors 1 – 4 were highly active for the polymerization of ethylene with controlled bimodal molecular weight distribution (MWD).

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발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 15:50, 좌장: 박강현

Enantioselective Iridium-Catalyzed Carbonyl Allylation, Crotylation and tert-Prenylation from the Alcohol or Aldehyde Oxidation Level

김인수

울산대 화학과

Existing methods for the enantioselective carbonyl allylation, crotylation and tert-prenylation typically suffer from the pre-activation associated with the use of chiral modifiers and the stoichiometric generation of pre-metallated nucleophiles. Under the conditions of transfer hydrogenation employing an ortho-cyclometallated iridium C,O-benzoate catalyst, highly enantioselective carbonyl allylations, crotylations and tert-prenylations are achieved in the absence of stoichiometric metallic reagents or reductants. Herein we describe how the union of carbonyl addition and hydrogenation chemistry has evoked a new suite of catalytic methods for enantioselective carbonyl allylation. Unlike classical methods for carbonyl allylation, the hydrogen-mediated variants occur in the absence of stoichiometric allylmetal reagents, minimizing or entirely excluding generation of stoichiometric byproducts. Additionally, under transfer hydrogenation conditions, alcohols may serve dually as hydrogen donors and aldehyde precursors, enabling carbonyl addition directly from the alcohol oxidation level, thus circumventing redox manipulations required for discrete generation of carbonyl electrophiles. These protocols are among the first methods available for direct catalytic C-H functionalization of alcohols at the carbinol position.

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발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 16:20, 좌장: 박강현

Assembled Organometallic Systems for Catalytic Applications

손성욱

성균관대 화학과

During the last decades, there has been great interest in preparation of the assembled materials such as metal-organic (MOFs) and covalent organic frameworks (COFs). Recently, the tailored functionalization of these materials has been an important subject for practical applications as gas storage materials, catalysts and etc. In this talk, the designed synthesis of MOFs and COFs bearing the imidazolium salts and relevant N-heterocyclic carbenes will be presented. Especially, this talk will focus on the following three issues. First, our research group recently disclosed the concomitant formation of NHC-metal species during the assembly process of MOFs. Second, the main-chain metallo-polymers have been prepared using the predesigned building blocks. Third, the designed and post-functionalized COFs bearing imidazolium salts have been successfully prepared and applied as green catalysts.

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발표코드: **ORGN/INOR-7**
발표분야: 유기/무기 공동심포지엄: 유기/무기화학과 촉매
발표종류: 심포지엄, 발표일시: 금 16:50, 좌장: 박강현

Pd-Catalyzed C-H Activation and C-C/C-N Bond Formations

윤소원

한양대 화학과

Since C-H bonds are ubiquitous in organic compounds and aromatic moieties are the most common structural motifs in natural products, pharmaceuticals, and organic materials, direct and catalytic C-H bond activation of aromatics would provide very efficient, economical, and environmentally friendly synthetic methods for chemical industries. A recent report in which C-H activation of aromatics has been identified as a key green chemistry research area of the most need for the industry as well as a continuously growing number of publications regarding C-H activation imply a prominent position held by this research area in the contemporary organic chemistry, making substantial progress during the last several decades.In this seminar, I will present the discovery of several efficient transformations via effective C-H activation and subsequent C-C/C-N bond formations. These synthetic methods provided mild, simple, and efficient routes to valuable functionalized arenes and heterocycles, which are important motifs in a number of natural and designed bioactive compounds and organic materials.

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장소: 대구엑스코
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발표분야: 염증성질환치료제의 개발동향
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이종국

Arvelexin isolated from the Brassica rapa abolishes inducible NF-κB activation by inhibiting IKK activation, thereby suppressing NF-κB-regulated pro-inflammatory gene expression

이경태

경희대 약학대학 약학과

Background and purpose: Brassica rapa species constitute one of the most important sources of food. In the present study, we investigated the anti-inflammatory effects and the underlying molecular mechanism of arvelexin, which was isolated from B. rapa as an active component, on lipopolysaccharide (LPS)-stimulated RAW264.7 macrophages and on carrageenan-induced paw oedema in rats. Experimental approach: Inducible nitric oxide synthase (iNOS) and cyclooxygenase-2 (COX-2), tumor necrosis factor-α (TNF-α), interleukin-6 (IL-6), and IL-1β expressions were determined by Western blot and/or RT-PCR, respectively. To elucidate the underlying mechanism, nuclear factor-kappa B (NF-κB) activation and its pathways were investigated by EMSA, reporter gene, and Western blot assays. In vivo anti-inflammatory effects of arverexin were evaluated in rat paw oedema induced by carrageenan. Key results: iNOS and COX-2 promoter assay revealed that arvelexin inhibited LPS-induced NO and PGE2 production through the suppression of iNOS and COX-2 at gene transcription levels. In addition, arvelexin inhibited NF-κB-dependent inflammatory responses by modulating a series of intracellular events of IκB kinase (IKK)-inhibitor κBα (IκBα)-NF-κB signaling. Moreover, arvelexin inhibited IKKβ-elicited NF-κB activation as well as iNOS and COX-2 expressions. Consistent with these results, treatment with arvelexin prevented the carrageenan-induced oedema formation and MPO activity in rats. Conclusion and implications: Arvelexin downregulates inflammatory iNOS, COX-2, TNF-α, IL-6, and IL-1β gene expression in macrophages by inhibiting the activation of NF-κB activation by interfering with the activation IKKβ and p38 MAPK.

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발표분야: 염증성질환치료제의 개발동향
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이종국

염증치료신약후보의 발굴 및 개발 (Discovery & Development of Anti-Inflammatory Drug Candidates)

노성구

크리스탈지노믹스(주)

During the last several years, we have focused on the discovery and development of anti-inflammatory drug candidates. The program includes clinical studies on CG100649, a next generation NSAID, and discoveries of novel inhibitors targeting inflammation related proteins. CG100649 inhibits COX-2 in a tissue-specific manner through the dual inhibition of COX-2 and carbonic anhydrase (CA). Namely, oral administration of CG100649 results in significant levels of free active drug in joints and synovial fluid which are devoid of CA activity, but it is sequestered in an inactive form in many other tissues because the drug is tightly bound to CAs, a known family of proteins that are prevalent in the blood and in sites of potential COX-2 toxicity. On the basis of such a unique mechanism, CG100649 showed clear efficacy and differentiated safety profiles from other NSAIDs in several clinical studies. To date, there were no serious adverse events and no indication of negative effects on the heart function, ECG profiles and blood pressure. Moreover, there weren't any evidence of gastrointestinal bleeding in any of the groups. CrystalGenomics' other anti-inflammatory projects are still in the discovery stage, but we have already obtained some compounds showing desirable efficacy and pharmacokinetic properties. In this presentation, the process and results of our progress will be discussed.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI-3**
발표분야: 염증성질환치료제의 개발동향
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이종국

Highly Potent IKKβ Inhibitors for Treating Rheumatoid Arthritis

신계정

KIST 생체과학연구본부

Nuclear transcription factor NF-κB plays a crucial role in the pathogenesis of multiple inflammatory diseases including rheumatoid arthritis. Inhibitory κB kinase-2 (IKKβ) is recognized to be a significant enzyme for activation of NF-κB signaling by phosphorylation of inhibitory κB (IκB) protein. Although IκB kinase is a multi-subunit kinase that contains two catalytic subunit as IKKα and IKKβ, it is generally accepted that IKKβ inhibition plays a more important role in regulating NF-κB sinaling transduction than IKKα. Therefore, IKKβ inhibitors with a selective binding property over IKKα and good efficacy are of interest as a small molecule drug for rheumatoid arthritis. Until now, there has been a lot of effort in the pharmaceutical industry finding out small molecule IKKβ inhibitor for inflammatory diseases. Here we will discuss the design and generation of novel, selective and potent IKKβ inhibitors. Also we will show in vivo animal data against CIA model.

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발표분야: 염증성질환치료제의 개발동향
발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 노은주

Inhibition of LXRalpha-dependent steatosis and steatohepatitis by licorice flavonoids

김상건

서울대 약학대학

Liver X receptor-alpha (LXRalpha) functions as a major regulator of lipid homeostasis through activation of sterol regulatory element binding protein-1c (SREBP-1c), which promotes hepatic steatosis and steatohepatitis. NF-E2-related factor 2 (Nrf2) is the crucial transcription factor that is necessary for the induction of anti-oxidant enzymes. This study investigated the potential of liquiritigenin (LQ) and isoliquiritigenin (ILQ), hepatoprotective flavonoids present in licorice, to inhibit LXRalpha-induced hepatic steatosis and steatohepatitis, and the underlying mechanism of the action. LQ treatment attenuated fat accumulation and lipogenic gene induction in the liver of mice fed high fat diet. Also, LQ had the ability to inhibit oxidative liver injury, as shown by decreases in thiobarbituric acid reactive substances formation and nitrotyrosinylation. Moreover, LQ treatment antagonized LXRalpha agonist (T0901317)-mediated SREBP-1c activation, and transactivation of the lipogenic target genes. LQ were found to activate Nrf2, and the ability of LQ to inhibit LXRalpha-mediated SREBP-1c activation was reversed by Nrf2 deficiency, which supports the inhibitory role of Nrf2 in LXRalpha-dependent lipogenesis. Consistently, forced expression of Nrf2 also inhibited LXRalpha-mediated SREBP-1c activation. In addition, the anti-steatotic effects of isoliquiritigenin (ILQ), another flavonoid in licorice, on the LXRalpha function and high fat diet animal model were observed as mediated by JNK1 inhibition. Our results demonstrate that LQ has an efficacy to activate Nrf2, which contributes to inhibiting the activity of LXRalpha that leads to SREBP-1c induction and hepatic steatosis.

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발표분야: 염증성질환치료제의 개발동향
발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 노은주

Stitching α-Helical Peptides: A Promising Approach to Next-Generation Anti-inflammatory Therapeutics

Young-Woo Kim

Harvard University

Many intracellular protein-protein interactions (PPIs) involved in inflammatory signal transduction pathways have proved highly promising as novel targets to treat inflammatory diseases. However, functional modulation of these intracellular PPIs using our two major drug modalities, namely small molecules and biologics, has been extremely challenging: PPIs lack well-defined hydrophobic binding pockets for small molecules, and the intracellular location of PPIs limits the use of biologics, which in general cannot penetrate cell membranes. We have previously developed a synthetic strategy, termed "peptide stapling," which enforces the α-helical conformation in synthetic peptides via an all-hydrocarbon staple and thereby endows the peptides with significantly enhanced helicity, thermal and chemical stabilities, protease stability, binding affinity for their targets, and most importantly, cellular uptake. As α-helices play a critical role in mediating many PPIs, the α-helical "stapled" peptides have successfully demonstrated their potential as a new type of drugs or probes that directly modulate intracellular PPIs involved in many important biological processes including inflammation.In this talk, I will discuss an advanced version of the peptide stapling system, termed "peptide stitching," based on highly regio- and stereoselective multiple ring-closing olefin metathesis reactions leading to tandem-stapled peptides having a central spiro ring junction, which even further improves the desirable properties of "stapled" peptides. Such well-blended pharmacologically attractive features of the "stitched" peptides warrant their further exploration as next-generation therapeutics for macromolecular targets currently considered "undruggable" in inflammatory signaling pathways.

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발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김점수

Prospective Organic Materials for Energy Storage Devices

최남순

울산과학기술대 친환경에너지공학부

Li-ion batteries are very attractive for applications in electric vehicles (EVs), hybrid electric vehicles (HEVs), and plug-in hybrid electric vehicles (PHEVs) owing to their high energy density and long lifetime. Unfortunately, thermal stabilities of main components of batteries are apprehensive to apply to the filed of large-scale power sources. Especially, carbonate solvents contributing to the dissociation of lithium salt are volatile, potentially combustible, and might lead to thermal runaway of batteries at any abuse condition. In this point of view, the challenges for development of nonflammable electrolytes are required to attain highly safe batteries. In this presentation, various analytical ways will be introduced to manifest the effect of electrolytes on thermal and electrochemical properties of electrodes, and intriguing approaches for nonflammability of electrolytes will be described. Moreover, we will focus on some of the most significant examples of recent key developments in nonflammable electrolytes. It should be noted that thermally resistive materials such as ionic liquids and flame retardants readily undergo the electrochemical reduction during lithium insertion into an anode and provoke the irreversible capacity of cells. Therefore, reducible additives on an anode are needed to suppress the reductive decomposition of nonflammable materials and to assure superior electrochemical performances of cells. Here, functional additives for the formation of robust SEI will be presented. We hope that this presentation will generate interest in the community and encourage the researchers to make use of advanced nonflammable materials in batteries.

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발표코드: **MAT1-2**
발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김점수

Structural Evolution of Layered $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$upon Electrochemical Cycling in a Li Rechargeable Battery

강기석

KAIST

$Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$, one of most promising candidate cathodes for next generation Li rechargeable batteries has been the subject of much recent investigation because of the exceptionally high capacity which exceeds the theoretical capacity based on conventional chemical concepts, since these materials were first introduced by Lu *et al*. The detailed cation ordering between Ni, Mn and Li in the transition metal layer of $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$ is not clear yet. However, it is believed that the abnormally high capacity is closely related to the initial structure of this material and the structural change occurring during cycles.The mechanism and the origin of the overcapacity have not been clearly identified yet. Though simultaneous oxygen evolution during the first delithiation was demonstrated previously by many authors, it may only explain the high capacity of the first charge process; the high capacity at subsequent cycles should be elucidated further. A number of researchers showed that the transition metal migration and reordering took place during the electrochemical cycling through various tools. However, despite these given information, it is not still clear how the overall structural evolution of $Li[Li_{(1/3-2x/3)}Ni_xMn_{(2/3-x/3)}]O_2$ occurs and what structure it evolves to.In this talk, the overcapacity mechanism and the structural evolution of $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$ during the electrochemical reaction are investigated through careful study of electrochemical profile analysis, ex-*situ* XRD, HR-TEM, Raman spectroscopy and first principles calculation.

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발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김점수

Energy Storage Materials: Nano, Crystal structure and Mechanism

이규태

울산과학기술대 친환경에너지공학부

The most successful cathode materials of rechargeable lithium batteries are layered lithium transition metal oxides with formula of LiMO2 (M: Co, Mn and Ni) that crystallize in a layered structure. This topology offers highly accessible ion diffusion pathways. However, these materials have limitations of safety and cost problems, resulting in demand of developing new cathode materials. Therefore, a new class of transition metal polyanion materials has attracted much attention as a potential candidate. The most prominent compound of this group studied to date has been LiFePO4, which crystallizes in the olivine structure. The major limitations of LiFePO4, namely poor electrical conductivity and one-dimensional Li-ion diffusion, have been largely overcome by adopting nanosized LiFePO4. However, little unequivocal quantification of “nano” effects has been provided owing to the difficulty of measuring them. 1) This presentation will discuss these factors in a range of lithium metal phosphate nanocrystallites, LiMPO4 (M = Fe, Mn). 2) Also, in the search for structural frameworks that overcome the 1-D ion conductivity challenge of olivine, the tavorite family of compounds with the general formula LiMXO4F (M = Fe, V; X = P, S) which crystallize in the triclinic space group P-1 will be discussed. 3) In addition, Li-Sulfur batteries will be introduced as a next generation system of Li batteries. 4) Finally, this presentation will introduce a new type of rechargeable Na batteries to overcome a shortage of lithium resources. The configuration of our Na batteries used Na metal as anode material and NaMPO4 (M = Fe, Mn) as cathode materials.

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발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 최남순

Current R&D Trends of Lithium Ion Capacitors

김점수, 김영준

전자부품연구원 차세대전지연구센터

리튬이온 커패시터는 초고용량 커패시터의 고출력, 장수명 특성과 리튬이온전지의 고에너지밀도 장점을 하나의 장치로 구현할 수 있는 융합형 차세대 에너지저장 장치로써 스마트카드, RF-ID, Mobile Phone, GPS, AMR, Wireless Lan, Sensor network node, Zigbee, Bluetooth 등의 용도로 제품 개발이 진행되고 있으며 최근 전 세계적으로 활발하게 연구개발이 진행되고 있는 스마트 그리드용 및 신재생 에너지용 에너지 저장 장치로의 응용도 고려되고있다. 리튬이온 커패시터는 활성탄계 양극, 복합 탄소계 음극, 유기계 전해액으로 구성되며 기존의 커패시터와는 달리 양/음극이 비대칭 특성을 보인다. 비대칭 특성의 주 인자는 음극 쪽에 사용되는 탄소 소재로 그 특성(전기화학적)의 차이가 커패시터의 특성에 직접적인 영향을 미친다. 본 연구에서는 리튬이온 커패시터 최근 연구 개발동향과 리튬이온 커패시터의 핵심 요소기술 중의 하나인 pre-doping 에 대한 여러 종류의 탄소별 특성을 평가하고 그 특성이 커패시터 성능에 미치는 영향에 대해 보고한다. 리튬이온 커패시터의 특성상 리튬이온 배터리에서 사용하는 음극재와 동종의 소재인 카본류에 대한 를 적용하였고 음극재의 종류에 따라 초기 비가역용량, 가역용량, 율특성 등이 차이가 나고 이 특성의 차이가 커패시터 cell 의 다양한 평가 시 발현되는 차이점에 미치는 영향을 3 전극 또는 4 전극 cell 을 이용하여 연구하였다.

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발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 최남순

Silicon Nanowire Anodes: Size Effect Studied in a Single Nanowire Resolution

최장욱

KAIST EEWS

Silicon has been most promising anode material due to its high capacity, ~ 4000 mAh/g, in Li ion batteries. However, it undergoes significant volume expansion during cycling and deteriorates cycle life because it pulverizes and lose physical contact with current collectors due to the volume expansion. In order to overcome this mechanical drawback, a variety of nanostructures have been suggested and demonstrated for remarkably improved cycle life. For deeper understanding of this advantage associated with small size, we develop unique TEM technique by which single identical silicon nanowires (Si NWs) can be traced during electrochemical reactions. Using this technique, the following size dependent phenomena were observed: 1. NWs with smaller diameters recover their original diameters after a full cycle of lithiation and delithiation, while NWs with larger diameters do not. 2. NWs with smaller diameters were affected by oxide layers on the surface and thus do not expand as much as those with larger diameters. Finally, these single nanowire based observations were applied to real battery cells. Analogous size effect was also observed in these large scales cells.

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발표분야: 리튬이차전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 최남순

Who will drive EVs, Olivine or Spinel?

송현곤, *조재필

*울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부*

Rechargeable batteries based on lithium ions have been maturely considered as the most dominant technology in the field of energy storage due to their high energy density. Since the lithium ion batteries (LIB) were introduced into market, the application targets are evolved from small mobile devices to large-scale applications including EVs and stationary energy storage wells. Obviously, hot concerns are devoted to EV applications of LIB. It must be one of the main issues to choose cathode materials in terms of energy density, power density (rate capability), cycle life (stability), safety and cost (material and process costs). Lithium manganese oxide with spinel structure (LMO spinel, $LiMn_2O_4$) and lithium iron phosphate with olivine structure (LFP olivine, $LiFePO_4$) are competitively being developed for the target field. LMO spinel and LFP olivine have their own merits relative to its counterpart when compared to each other. We believe that it is the time to review those strongest candidates as cathode materials for electric vehicles. Merits and demerits of their intrinsic properties will be compared and then how to overcome the demerits will be discussed. It will be concluded with what would be a practical solution or direction for the near future.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MAT2-1**
발표분야: 최신 나노위해성 연구 동향
발표종류: 심포지엄, 발표일시: 금 09:15, 좌장: 양성익

Current limitations and challenges in the toxicity assessments of manufactured nanomaterials

윤태현, 권동욱, 박재홍, 이송희

한양대 화학과

Due to the increasing concerns on the potential risk of manufactured nanomaterials, understanding their toxicity mechanism, environmental fates, and impacts on human health and ecosystems became one of the urgent scientific issues to be addressed. Here, based on our recent studies on the TiO2, nano-Ag etc., current limitations and challenges in nanoparticle toxicity assessments will be discussed. Particularly, among the many issues of nanoparticle toxicology, we will focus on the issues of the appropriate dosing metrics of NPs and effects of various physicochemical properties on the dosing metrics as well as the limitations of current cytotoxicity assay protocols for the assessment of NP toxicity

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장소: 대구엑스코

발표코드: **MAT2-2**

발표분야: 최신 나노위해성 연구 동향

발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 양성익

나노 물질의 위해성 평가 기준안 마련시 고려할 사항

김준성

바이테리얼즈

나노물질에 대한 생체 유해성을 평가하기 위하여 나노물질의 물리 화학적 특성평가를 위한 표준 측정 기술 및 분석 기술을 정립하고 다양한 관점에서 독성 발현에 관한 정밀한 연구를 진행하여 유해성 평가 표준안을 확립한다

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MAT2-3**
발표분야: 최신 나노위해성 연구 동향
발표종류: 심포지엄, 발표일시: 금 10:05, 좌장: 양성익

Label-free Mass Imaging of Nanoparticles for Nanosafety

이태걸, 송남웅, 문대원, *신승구

*한국표준과학연구원 미래융합기술부 나노바이오융합연구단 *포항공과대 화학과*

Studies of nanoparticles have exponentially increased due to their potential in various applications in the bio-industry. The great advances in nanoparticle synthesis have especially increased the possibility of incorporating these nanoparticles into our daily lives. Although nanoparticles have a variety of potential applications, there are still the toxicity and biocompatibility problems to resolve before applying them to biology and medicine, which underscores the need to understand the movement mechanism and distribution of nanoparticles *in vivo*. In this talk, we will show that label-free mass imaging analysis technique would be helpful to understand *in vitro* and *in vivo* cytotoxicity of nanoparticles [1-3].[1] H.K. Shon, et al., J. Nanosci. Nanotech. 2010, in press[2] H.K. Shon, et al., Surf. Interf. Anal. 2010, in press[3] H. Min, et al., Chem. Eur. J. 2008, 14, 8461-8464

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장소: 대구엑스코
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발표분야: 최신 나노위해성 연구 동향
발표종류: 심포지엄, 발표일시: 금 10:45, 좌장: 윤태현

Development of Nanomaterial Characterization Methods for Safety Evaluation

송남웅

한국표준과학연구원 미래융합기술부 나노바이오융합연구단

Commercialized products based on nanomaterials are increasingly launched to the market along with the development of the nanotechnology. It is prerequisite to validate the safety of those products on the environment and human health to be distributed in the market. For the toxicity test or study on the interaction with living bodies, the physicochemical properties of nanomaterials should be characterized by using reliable analysis techniques. However, the measurement methods for some characteristics have to be developed to give consistent, quantitative and accurate results. In the "Center for Nanobio Technology" in KRISS, we are seeking reliable methods to identify various kinds of nanomaterial characteristics that include size, size distribution, surface charge/composition, optical and photoinduced chemical properties. We are also trying to relate the interaction behavior of nanomaterials with their physicochemical properties at cellular level.In this presentation, some examples of nanomaterial characterization methods by using microscopic and spectroscopic techniques, which are being developed in KRISS, will be introduced. These techniques include, 1) Single particle analysis for the characterization of optical property and surface states of fluorescent nanoparticles 2) Uncertainty evaluation of the nanoparticle size distribution 3) Surface characterization methods for the synthesized and purified nanoparticles 4) Stabilizing the TiO2 nanoparticle suspension and multiplexed assay method for its photocatalytic activity.

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발표분야: 최신 나노위해성 연구 동향
발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 윤태현

Live-cell imaging and tracking of intracellular nanoparticles for the safety issues

주상우

숭실대 화학과

Understanding the endocytosis and intracellular accumulation mechanisms of nanomaterials in live cells could lead a better assessment of their toxicity issues. Real time particle tracking is an important tool for studying cellular processes that involve molecular motilities. The information obtainable from the acquired trajectories is often determined to investigate dynamic biological processes by following individually labeled molecules' movements with instrumental resolution. Live-cell imaging is one of the most useful techniques for performing real time studies of the interactions among biological molecules in living cells. Fluorescence nanomaterials have been utilized as one of the most efficient tools for this purpose because of their superior sensitivity and selectivity. On the other hand, surface enhanced Raman scattering (SERS), an ultra sensitive spectroscopic tool for interface studies, has been widely used for biological sensing or molecular imaging near the surface of nanostructure assemblies to overcome the photo-bleaching effects of fluorescence measurements. The SERS method offers several advantages due to different Raman signatures for labeling various biomolecules with narrow bandwidths to avoid spectral overlaps. Our preliminary results will be discussed at the symposium.

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장소: 대구엑스코
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발표분야: 최신 나노위해성 연구 동향
발표종류: 심포지엄, 발표일시: 금 11:35, 좌장: 윤태현

Graphene: Cytotoxcity and Cellular Response

민달희

KAIST 화학과

Graphene and graphene derivatives have attracted enormous attention from various research fields for applications in electronic devices, transparent electrodes, biosensors, drug delivery system and surface coatings. In the viewpoint of chemist, the chemical structure of graphene derivatives seems intriguing but detailed structures are being revealed only recently while engineering approaches for various applications are being executed very actively. In addition, cytotoxicity and mammalian cellular responses to graphene have not thoroughly investigated yet in spite of the importance in bio-applications and environment. In this talk, I'll introduce recent studies which report cytotoxicity and behaviors of mammalian cells when the cells exposed to graphene (as well as some bio-applications of graphene), especially to get closer to answers to these questions, "how we understand and how/why we use graphene".

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 명노승

Photo-induced Electron Transfer Reactions Occurring on Modified Titania Surface for Simultaneous Production of H2 and Degradation of Organics

최원용, 김정원

포항공과대 환경공학부

Semiconductor photocatalysis has been extensively studied for the synthesis of solar fuels such as hydrogen and the degradation of pollutants. Although both applications are based on the same principle of the photoinduced electron transfers, achieving the dual purpose photocatalysis (i.e., simultaneous production of hydrogen and degradation of water pollutants) remains a challenging issue. In this talk, the surface of TiO2 nanoparticles was modified by simultaneous surface fluorination and platinization and the surface-modified photocatalysts were successfully demonstrated for the simultaneous production of hydrogen and degradation of organic compounds (particularly phenolic compounds) in water. The surface platinization and surface fluorination of TiO2 have been studied independently and each modification method influences the photocatalytic activity in very different ways. The synergistic effect of two different surface species can exhibit the anoxic degradation of organic compounds. Furthermore, the simultaneous modification can highly improve the hydrogen production in the presence of phenolic compounds. Highly synergistic effect of surface fluorination and platinization of TiO2 is related to the substrate-surface interaction and the charge transfer/recombination processes. The production of hydrogen gradually decreased as the organic compounds were depleted. The dual purpose photocatalysis was also confirmed under sunlight irradiation and can be developed to a solar conversion technology that achieves hydrogen production and water treatment simultaneously.ch

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 명노승

New Concept of Highly Efficient Dye-Sensitized Solar Cells

고재중

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). The 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 issues, we proposed a new route to assemble CdSe QDs onto TiO2 films in this study.

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 명노승

Flexible Electrochromic Film Devices Based on Nanoparticles of WO_3, Prussian Blue and Prussian Blue Analogues

김영일, *곽준영, 정영희

*부경대 화학과 *부경대 화학과/(주)마프로 연구소*

Although electrochromic devices have huge potential as dynamic glare/heat control devices for architectural and automotive applications, e.g. smart windows, the commercialization of such products is far from reaching their potential. Making the durable large-area devices cost-effectively is still challenging. We have developed a technology of roll-to-roll processing of electrochromic films on PET/ITO substrate. Utilizing silica sol mixed with electrochromic nanoparticles such as nanocrystalline WO_3, Prussian blue (PB) and Prussian blue analogues (Ni-PBA and Cu-PBA), very effective and durable electrochromic film electrodes have been prepared by wet-coating methods. In this presentation the electrochromic electrodes of PET/ITO/WO_3, PET/ITO/PB, PET/ITO/Ni-PBA and PET/ITO/Cu-PBA and the electrochromic devices prepared from the combination of two of them with polymer-gel electrolytes will be discussed.

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김종원

2차 염료흡착을 통한 고전류 특성 병렬탠덤구조 염료감응 태양전지

전용석, *한치환, **강만구

*울산과학기술대 *한국에너지기술연구원 광전기소재연구센터 **한국전자통신연구원*

염료감응 태양전지는 다른 태양전지에 비하여 저렴한 가격과 단순한 공정 그리고 우수한 출력으로 지난 수년간 많은 주목을 받아왔다. 하지만 염료감응 태양전지에서 주로 전력을 생산하는 부분인 감광성 염료는 제한적인 태양광 흡수단을 가지므로 더 높은 효율을 보이기 위해서는 더욱 폭넓은 흡수단을 가지는 염료의 필요성이 대두되어왔다. 그리하여, 많은 연구를 통하여 다양한 구조를 가지는 염료가 개발이 되었는데, 이런 염료를 활용하여 더욱 넓은 범위의 태양광을 흡수하는 탠덤구조의 염료감응 태양전지는 지금까지도 꾸준히 연구되어 오고 있다. 본 연구에서는, 1 차 자리조립된 염료와, 염료사이 사이의 빈자리에 크기가 작은 다른 염료를 2 차적으로 침투 및 흡착시켜 하나의 전극에서 좀 더 높은 동작특성을 구현할 수 있는 병렬탠덤구조 염료감응 태양전지를 제안하고자 한다. 이렇게 제조된 전지의 특성을 전압의 변화와 전류값, 임피던스 등을 통해 분석하였다. 본 연구에서 사용된 2 차염료 이외의 더 좋은 효율을 보이는 염료가 개발이 되어 활용된다면 더욱 향상된 효율을 보여줄 수 있을 것으로 기대된다.

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 김종원

Electrochemistry in DSSC: THE ROLE OF INTERHALOGEN BASED REDOX COUPLE for High voltage DSSC

이재준

건국대 응용화학과

A novel electrolyte system with an interhalogen based novel redox system was developed for higher open circuit voltage of dye-sensitized solar cells (DSSCs). It was found that the interhalogen ions, I2Br- can be formed by electrochemically as well as by chemical equilibrium. The redox reaction involved with these ions is comparable to that of electrochemical oxidation of iodide to triiodide in the conventional DSSC, but it occurred at a more positive formal potential than that of the former. The formation of these extra redox states at more positive potential than I-/I3- couple contribute to increase the open circuit voltage of DSSCs regardless of dyes by shifting positively the equilibrium potential of solution phase. Furthermore, this equilibrium potential could be controlled by adjusting the concentration of these redox species in the solution.

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발표분야: 광변환전지의 현재와 미래
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 김종원

Photoanodes of DSSCs for low-temperature processes

표명호

순천대 화학과

No involvement of a high-temperature sintering procedure for TiO2 films excludes the usage of polymeric binders. This inevitably leads to difficulties in the formation of inter-particle connections between TiO2 and the control of pore sizes, which results in slow electron transport through TiO2 films and/or inconsistent I3- diffusion through an electrolyte medium. To circumvent this barrier, various strategies such as incorporation of TiO2 nanotubes,mechanical compression of TiO2 films, and electrophoretic deposition of TiO2 have been reported via a low-temperature process. Despite the importance of TiO2 nanostructures in a low-temperature process, no previous work has investigated the effect of TiO2 composition on the performance of low-temperature DSSCs. This may be because it was assumed that the optimal TiO2 composition made through a high-temperature process was also valid for low-temperature DSSCs. That is not the case, however, since TiO2 made at a low temperature possesses loosely-interconnected TiO2 and thereby inferior electron transport properties. From this regard, the optimization of nanostructures for low-temperature TiO2 may be more important than that for high-temperature TiO2. In this work, we will present the new strategy which can optimize TiO2 nanostructures and be applied the continueous printing process at low temperature.

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발표코드: **ENVR1-1**
발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 박현웅

Synthesis of Nanomaterials for Electrochemical Energy Conversion

박경원

숭실대 환경화학공학과

The physical, electrochemical, electronic, and optical properties of nanostructured materials are well known to be different from those of bulk materials. In particular, nanostructured metal and/or oxide can have significantly enhanced electrochemical reaction rates over those of bulk materials. Hence, well-designed nanostructures are essential for the preparation of electrodes for use in electrochemical power sources such as fuel cells, solar cells, and batteries.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **ENVR1-2**
발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 박현웅

LUTEIN CAN ACT AS A SWITCHABLE CHARGE-TRANSFER QUENCHER IN A LIGHT-HARVESTING COMPLEX

안태규

성균관대 에너지과학과

Energy-dependent quenching of excitons in Photosystem II of plants, or qE, has been positively correlated with the transient production of carotenoid radical cation species. Zeaxanthin was shown to be the donor species in the CP29 antenna complex. We report transient absorbance analyses of CP24 and CP26 complexes that bind lutein and zeaxanthin in the L1 and L2 domains, respectively. For CP24 complexes, the transient absorbance difference profiles give a reconstructed transient absorbance spectrum with a single peak centered at ~980 nm, consistent with zeaxanthin radical cation formation. In contrast CP26 gives constants for the decay components probed at 940 nm and 980 nm of 144 ps and 194 ps, a transient absorbance spectrum that has a main peak at 980 nm, and a substantial shoulder at 940 nm. This suggests the presence of two charge-transfer quenching sites in CP26 involving zeaxanthin radical cation and lutein radical cation species. We also show that lutein radical cation formation CP26 is dependent on binding of zeaxanthin to the L2 domain, implying that zeaxanthin acts as an allosteric effector of charge-transfer quenching involving lutein in the L1 domain.

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발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 박현웅

TiO_2 nanofibers as a efficient photocatalysts

김순현

대구경북과학기술원 나노바이오연구부

Nanostructured TiO_2 and mesoporous TiO_2 have been reported to have novel properties and application fields with improved performances. Nanostructure has intrinsically different energetics and electrochemical properties, while mesoporosity increases the surface adsorption capacity of reactants as well as charge separation efficiency. In this study, we synthesized the TiO_2 nanofibers (TNF) by electrospinning of polymer solution containing nanosized TiO_2 particles prepared by sol-gel method. TNF had a diameter of around 500 nm was composed of ca. 30 nm-sized anatase and rutile particles which were densely packed together. The photocatalytic hydrogen production rate, the photocatalytic degradation kinetics of model substrates, and the photocurrent generation are significantly enhaced. These enhancements are likely to be ascribed to mesoporosity created by cavities among the TNF along with increased surface area, as well as inhibited electron-hole pair recombination as revealed by a photoluminescence study.

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발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 김순현

Environmental Application and Implication of C60 Fullerenes: Novel Photocatalyst vs Emerging Contaminant

이재상

KIST 환경본부/물환경센터

C60 and its derivatives display unique photochemical properties relevant to generation of reactive oxygen species (ROS). Since such ROS production is achievable with visible light and the oxidants are capable of organic pollutants oxidation and microbial inactivation, C60 and its analogues recently have drawn attention as promising photocatalyst. In an effort to use C60 fullerene-based photocatalytic system for water treatment and disinfection processes, diverse water-soluble C60 adducts were synthesized and their photochemical and antimicrobial properties were investigated. As a new strategy to enable practical application of C60-related materials, immobilization of C60 derivatives on silica support was suggested and applicability of C60-derivatized silica photocatalyst was assessed in terms of 1) visible light-induced 1O2 generation, 2) recycle and repeated use, and 3) pollutant degradation and viral inactivation. ROS generation by C60 under visible light irradiation and its possible aqueous availability combined could be at the center of concerns in environmental impacts of C60-based nanomaterials. In order to better understand behavior of C60 released in the environment, photochemical properties of aqueous C60 cluster, critical in eco-toxicological activity, were elucidated and comparative kinetic studies on ROS generation were carried out regarding C60 colloids with different aggregation degrees. It is highly probable that C60 aggregates can react with artificially introduced and naturally occurring oxidants and undergo associated chemical transformations. Oxidative degradations of C60 clusters under UV irradiation and by OH radical in water and the consequent chemical conversions were investigated through a suite of analytical techniques including TEM, XPS, ATR-FTIR, and MALDI-MS.

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발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 김순현

The influence of iron speciation on the reduction of Fe-DFOB siderophore complex

김동욱

육군사관학교학교 화학과

Siderophores are low molecular weight chemical compounds excreted by plants or microbes for the uptake of iron in iron-deficient environments. Siderophores form FeIII chelation complexes with exceptional stability (e.g., log beta > 30). To release iron metal center from Fe-siderophore complexes, it is necessary to reduce iron center by physiological reducing agents. However, reported values of reduction potential of reducing agents (e.g., NADH, FMN and FAD) *in vivo* cells are much higher than those of Fe-siderophore complexes. Thus, a great deal of work has examined the mechanisms of ferrisiderophore reduction. This study examines the reduction of FeIII complexes with DFOB (desferrioxamine B), a trihydroxamate siderophore, by the fully reduced hydroquinone form of flavin mononucleotide (FMN_{HQ}). Our preliminary works have discovered that the oxidation of Fe-ligand complexes in homogeneous aqueous solution is strongly dependent on the iron speciation. Experimental results in this study also demonstrate that the rate and extent of FeIII-DFOB reduction is strongly dependent on solution conditions which is strongly correlated with iron speciation. Three independent processes observed in Fe, DFOB and FMN containing system and the correlation between the rate of reaction and iron speciation will be discussed.

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발표분야: 환경에너지 분야의 신진과학자
발표종류: 심포지엄, 발표일시: 금 16:40, 좌장: 김순현

Activation of oxygen and hydrogen peroxide by iron and its application for water treatment

이창하

울산과학기술대 도시환경공학부

Zero-valent iron (ZVI, Fe0) can activate oxygen into strong oxidants capable of decomposing various organic contaminants in water. However, the applicability of this approach to treatment is limited by the low yields of oxidants. Recently, a couple of attempts have been made to improve the efficiency of the oxidant production from ZVI. Introduction of nickel to ZVI (synthesis of bimetallic nickel-iron nanoparticles) enhanced yields of oxidants produced from ZVI by approximately two times under neutral pH conditions. Polyoxometalate (POM) greatly increased the oxidant yields of the system (approximately 4–6 times) by serving as an electron shuttle and an iron-chelating agent. The coordination of iron by POM also enhanced the reactivity of the oxidant by altering the mechanism of the Fenton reaction. In addition, nanoparticulate ZVI showed a strong biocidal activity against both bacteria and viruses, implying that ZVI can serve as a potential disinfectant or anti-biofouling material. Further research topics will be discussed for the effective application of ZVI and other iron-based technologies to water treatment.

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발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 김동하

METAL OXIDE/CARBON NANOCOMPOSITES FOR HIGH POWER ENERGY STORAGE APPLICATIONS

김광범

연세대 신소재공학과

Lithium-ion batteries are widely used for portable electronic devices such as cellular phones, notebook computers and portable recorders due to their high capacity, high voltage, portability and long cycle life. However, their new applications require both high rate capability and high capacity as in electrical and hybrid vehicles.Nano-sized metal oxides are expected to improve the high rate capability of cathode materials for lithium-ion batteries because of the considerably higher effective interfacial area between the nano-sized metal oxide and electrolyte, and its shorter lithium diffusion length during charge/discharge.[1] Similarly, nano-sized metal oxides are expected to improve the high rate capability of oxide-based electrode materials for supercapacitors. Since nano-sized metal oxides tend to agglomerate, good dispersion and improved conductivity of an electrode composed of nano-sized oxides is very important for achieving high rate capability.[2]Carbon nanotubes (CNTs) can act as good additives to disperse nano-sized metal oxides and connect them with a 1-dimensional conduction path. CNTs have chemical stability, good conductivity and large surface area. In addition, CNTs are strongly entangled, providing a network of open mesopores. CNT as an additive can improve the high rate capability of nano-sized metal oxides.3-5 Porous entangled structure of CNTs provides the interconnected pore structure for easy access of lithium ions to reaction sites. Increased contact area between nano-sized metal oxides and CNTs can improve the electric conductivity of the electrode. In addition, CNTs have a long conduction path on the μm scale.In this study, metal oxide/Nanocarbon nanocomposite materials ($LiMn_2O_4$/CNT, $LiMn_2O_4$/Graphene, $LiCoO_2$/CNT, $LiCoO_2$/Graphene, $Li_4Ti_5O_{12}$/CNT and $Li_4Ti_5O_{12}$/Graphene, Co_3O_4/graphene nanocomposites) were synthesized through selective heterogeneous nucleation and growth of the oxides on nanocarbon surface. In the composites, nanocarbons acted as a substrate to deposit nano-sized metal oxide and to connect the nanoparticles along a conduction path. The nano-

hybrid materials showed excellent high rate capability and good structural reversibility for energy storage applications.*References*(1)Arico, A.S.; Bruce, P.; Scrosati, B.; Tarascon, J.M.; Schalkwijk, W.V. Nat. Mater., 2005, 4, 366.(2)Jiang, C.; Ichihara, M.; Honma, I.; Zhou, H.; Electrochim. Acta, 2007, 52, 6470. (3)Ma, S.B.; Nam, K.W.; Yoon, W.S.; Yang, X.Q.; Ahn, K.Y.; Oh, K.H.; Kim, K.B. J. Power Sources, 2008, 178, 483.(4)Ma, S.B.; Ahn, K.Y.; Lee, E.S.; Oh, K.H.; Kim, K.B. Carbon, 2007, 45, 375. (5)Ma, S.B.; Nam, K.W.; Yoon, W.S.; Bak, S.M.; Yang, X.Q.; Cho, B.W.; Kim, K.B. Electrochem. Commum., 2009, 11,1575.(6)Ma, S.B.; Kim, K.B. in preparation

대 한 화 학 회
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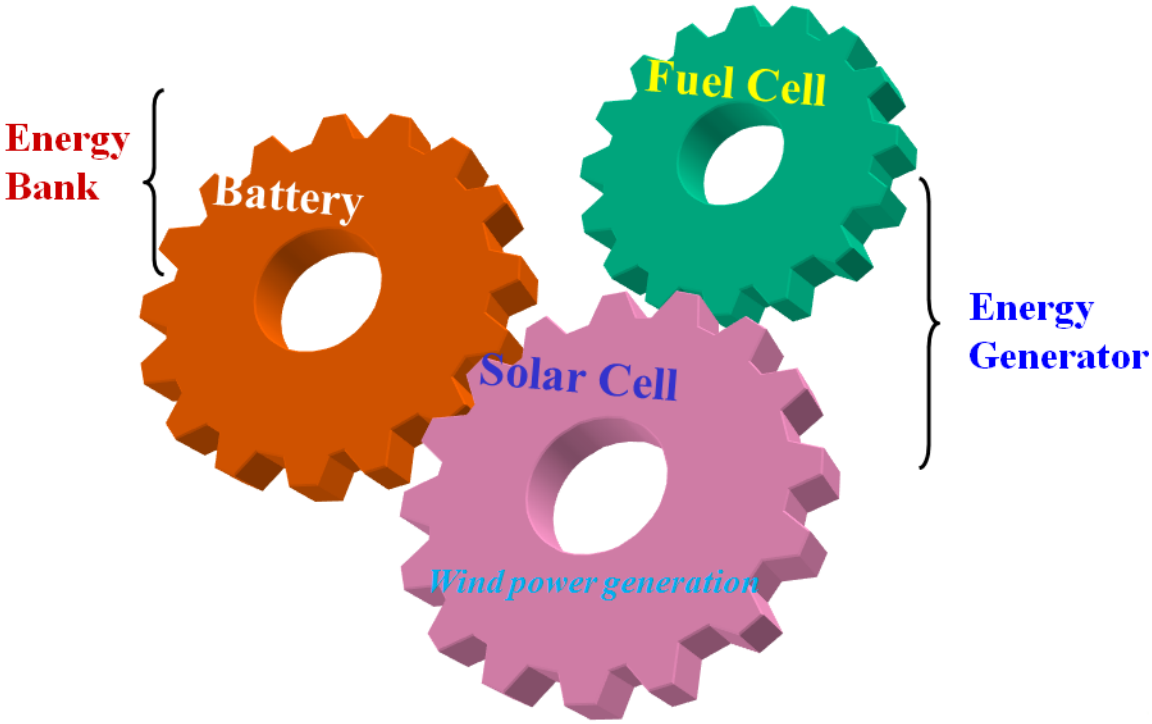
장소: 대구엑스코
발표코드: **ENVR2-2**
발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 김동하

Rechargeable Batteries in Hybrid Technology Era

조원일

KIST 에너지본부

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. Large size batteries, like redox flow battery, and sodium sulfur battery, have been developed as energy storage devices and lead acid batteries has been demonstrated as mega-watt range energy storage device. Now novel attempts are tried to make MW level rechargeable lithium battery systems in order to increase energy efficiency. In this talk, several kinds of rechargeable battery systems are reviewed and compared in a sense of economy.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ENVR2-3**

발표분야: 환경에너지 융합기술의 최신 동향

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김동하

화학적 수소저장 기술 개발 동향

남석우

KIST 연료전지센터

화학수소화물을 이용한 수소저장 방법은 고용량의 수소저장이 가능하고, 수소 방출이 실온에서도 가능하여 소형 연료전지 발전시스템에 매우 유용하다. 지금까지 NaBH4 및 NH3BH3 을 이용한 수소저장 기술에 대해 많은 연구가 있었으며, 최근에는 무인항공기 등 장시간 연속 구동이 필요한 연료전지 전원에 적용하여 실증 실험이 이루어지고 있다. 본 발표에서는 NaBH4 및 NH3BH3 을 이용한 화학적 수소저장 기술에 대해 최근 기술 동향을 알아본다. 특히 최근 국내 연구진에 의해 급진전이 이루어지는 수소방출용 유기금속촉매 및 나노촉매에 대해 자세히 알아본다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ENVR2-4**
발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 표승문

Photocatalytic and photoelectrochemical solar hydrogen production

이재성

포항공과대 화학공학과

Sunlight is a clean, renewable and abundant energy source on the earth. Its conversion to hydrogen has been considered an ideal solution to counter the depletion and environmental problems of fossil fuels. Photoelectrochemical water splitting is an ideal technology for the purpose, since H2 could be produced directly from abundant and renewable water and solar light from the process[1]. The key to the technology is photoelectrodes of high efficiency, high stability, and low cost. In addition of the discovery of new materials, the structure and morphology of the known materials could be designed to enhance the performance of the photoelectrodes. In this presentation, the concepts of materials design and their examples are proposed for efficient photoelectrodes of photoelectrochemical (PEC) cells for visible light water splitting. We discuss the material designs including: i) Nanoparticles electrodes to minimize the diffusion length of the minority carrier, ii) p-n heterojunction photoanodes for effective electron-hole separation, iii) electron highway to facilitate interparticle electron transfer, iv) metal doping to improve conductivity of the semiconductor, and v) one-dimensional nanomaterials for vectoral electron transfer. High efficiency has been demonstrated for all these examples due to efficient electron-hole separation. Modern material processing techniques have been explored to materialize these concepts [2-4]. [1] J.S. Lee, Catal. Surv. Asia 9 (2005) 217;[2] H.G. Kim, P.H. Borse, W. Choi, J.S. Lee, Angew. Chem. Inter. Ed. 117 (2005) 4661[3] H.G. Kim, E.D. Jeong, P.H. Borse, S. Jeon, K. Yong, J.S. Lee, W. Li, S.H. Oh, Appl. Phys. Lett. 89 (2006) 064103/1: [4] P.H. Borse, H. Jun, S.H. Choi, S.J. Hong, and J.S. Lee. Appl. Phys. Lett. 93 (2008) 17310.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ENVR2-5**
발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 표승문

태양전지 소재기술 동향

문상진

한국화학연구원 에너지소재연구센터

태양광을 전기 에너지로 바꾸는 태양전지는 차세대 대체 에너지원으로서 가장 주목을 받고 있는 소자이다. 고유가와 친환경성에 기인하여 세계 태양전지 시장은 21 세기 들어 매년 최소 30% 이상의 급신장세를 보여주며 2009 년 설치량 7.3 GW 에 360 억불 정도의 큰 산업으로 성장하였는데, 이로 인해 실리콘 소재의 수급 불균형에 따른 큰 가격 등락 등 부작용도 만만치 않았다. 현재 태양전지 산업의 주류를 차지하고 있는 결정질 실리콘 태양전지는 이러한 웨이퍼 기반의 높은 재료 가격으로 인해 제조단가가 여전히 높다. 따라서 최근들어 박막 기반의 무기, 유기 박막 태양전지에 대한 연구개발과 산업화가 크게 활기를 띄고 있으며, 실리콘 및 기타 다양한 태양전지 신소재에 대한 관심도 부쩍 증대되고 있다. 본 발표에서는 앞으로도 상당 기간 태양전지 산업의 주도적인 소재로 활용될 실리콘 소재를 비롯하여, 차세대 유기태양전지의 중요 핵심소재에 이르기까지 태양광 소재기술의 최신 동향을 살펴보고자 한다. 또한 태양광을 활용하는 물분해 광촉매 기술 등 연관 유사 기술의 동향도 간략히 덧붙인다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ENVR2-6**
발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 표승문

Methodology to Improve Light Harvesting and Charge Collection Efficiencies in DSSC

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, the redox electrolyte and the Pt counter electrode, where charge is generated by dye, TiO_2 film acts as both charge separation and electron transport, and redox electrolyte play the role in dye regeneration. 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 and charge collection efficiency is also important in terms of overall conversion efficiency. In this talk, nano-engineering technologies to have high light harvesting and charge collection efficiencies in DSSC will be presented.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ENVR2-7**
발표분야: 환경에너지 융합기술의 최신 동향
발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: 표승문

Low Cost, Printable High Efficiency Polymer Solar Cells

이광희

광주과학기술원 신소재공학과

Polymer bulk heterojunction (BHJ) solar cells based on composites of an electron-donating conjugated polymer and an electron-accepting fullerene offer promise for the realization of a low-cost, printable, portable and flexible renewable energy source in the near future. Through rigorous efforts in the improvement of the associate materials and the device science over the past decade, encouraging progress has been made with power conversion efficiencies (h_e) over ~6% in polymer BHJ solar cells. In this talk, I present here an innovative approach that significantly extends the device lifetime and at the same time enhances the device performance in polymer solar cells. By introducing a novel solution-based titanium oxide (TiO_x) layer between the active layer and the aluminum cathode in polymer BHJ solar cells, we demonstrate devices with excellent air stability and with enhanced performance. The TiO_x layer acts as a shielding and scavenging layer which prevents the intrusion of oxygen and humidity into the electronically active polymers, thereby improving the lifetime of unpackaged devices exposed to air by nearly two orders of magnitude. Moreover, we also demonstrate that this TiO_x layer enables us to fabricate 'all-solution processed' polymer tandem cells with a power conversion efficiency of 6.5%. The TiO_x layer is used to separate and connect the front cell and the back cell. The TiO_x layer serves as an electron transport and collecting layer for the first cell and as a stable foundation that enables the fabrication of the second cell to complete the tandem cell architecture. Our tandem cell architecture ensures the promise of high performance printable polymer solar cells with a significant extent of the range of possible applications.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDCOMM-1**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 최병순

사범대학 재학생과 졸업생의 반성적 글쓰기를 통해 살펴본 예비 화학 교사 교육의 장점과 개선점

한재영

충북대 사범대학 화학교육과

대부분의 화학 교사는 사범대학 졸업, 교육대학원 졸업, 일반대학의 교직이수 등을 통해 교사 자격증을 획득한 후, 임용고시(중등교사임용후보자선정경쟁시험)를 거쳐 국·공립 중등학교로 발령받거나 추가적인 모집 전형을 거쳐 사립 중등학교에 근무하게 된다. 이중 사범대학은 예비 교사 교육을 위한 목적대학으로서, 화학 교사 자격증 수여를 위한 기본 교육과정으로 교양, 교직, 전공(교과교육 및 내용학), 실습 등을 제시하여 운영하고 있다. 사범대학의 예비 화학교사들은 이러한 정규 교육과정을 이수할 뿐 아니라, 학과의 다양한 모임과 행사, 동아리, 봉사 등 여러 활동을 경험하며 미래의 화학 교사가 되기 위한 준비를 한다. 이 연구에서는 사범대학 재학생과 졸업생이 사범대학 화학교육과 대학생활에서 경험한 내용을 반성하여 글쓰기한 내용을 분석한다. 사범대학 대학생의 삶과 생활이 어떠한 모습으로 이루어지고 있는지 기술하고, 화학 교사 교육을 위한 대학으로서 사범대학의 장점과 개선할 점을 논의한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDCOMM-2**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 최병순

사범대학 재학생의 면담과 교육 만족도 조사를 통해 살펴본 사범 교육의 현주소

채희권

서울대 화학교육과

1996 년 교육개혁위원회에 의해 처음으로 교원양성기관 평가제도의 도입이 제안된 이래 전체 교원양성기관 유형별로 주기적이고 계속적인 평가가 실시되었다. 금년도는 제 3 주기의 첫해로서 전국 사범대학 화학교육 관련학과들을 대상으로 서면평가, 강의평가 및 교육수요자 만족도 조사 결과를 마친 상태이다. 이중에서 사범대는 재학생과 졸업생의 만족도 조사를 5 월 자체적으로 조사하였고 연구자는 기말고사 기간 중 3 학년 대상으로 면담을 실시하였다. 이러한 조사 내용을 통해 예비교사들의 현 사범교육제도에 대한 인식의 한 단면을 살펴보고 예비교사의 고민을 현 제도와 대비시켜 보고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDCOMM-3**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 최병순

예비화학교사를 위한 과학글쓰기 교육은 어떻게 이루어져야하는가?

남정희

부산대 화학교육과

교원양성대학의 교육과정이 개정되면서 과학논술이라는 과목이 도입되었다. 이미 여러 대학에서는 이 과목이 개설되어 시행되고 있으나 어떤 내용을 포함시켜야 할 것인지에 대해서는 교수자들이 많은 고민을 하고 있는 것으로 보인다. 예비교사들은 학교 현장에 나가 개정 교육과정에서 강조되고 있는 '과학글쓰기'를 가르쳐야 한다. 따라서 교원양성과정에서는 이들이 이를 가르칠 수 있도록 준비시켜야하는 실정이다. 이 발표에서는 예비교사들을 위한 과학논술 과목에 어떤 내용들이 포함되어야하면 어떤 방식으로 도입되어야 할 지에 대해서 다루고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDCOMM-4**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 차정호

화학교육과 실험교육의 현실과 나아가야할 방향

정대홍

서울대 화학교육과

화학교육과에 입학한 학생은 졸업하기까지 다수의 실험교과목을 이수한다. 각 대학마다 차이가 있을 것이고 개설되는 강좌명이 동일하지는 않겠지만, 일반화학실험, 물리화학실험, 유기화학실험, 무기화학실험, 분석화학실험, 중등과학실험 등이 전부 또는 부분적으로 포함될 것이며, 물리, 생물, 지구과학 영역의 교과 이수 중에도 실험강좌를 이수하게 된다. 이렇게 많은 실험을 이수하면서 학생들은 실험에 대한 전문성이 얼마나 향상될까? 개별 교과목의 교수자로서가 아니라 사범대학의 교육자로서 4 년의 실험교육을 통해서 학생들에게 기대하는 전문성은 무엇인가? 4 년의 실험교육의 목표는 어떤 방법으로 개별 실험강좌에 반영되어 추진되고 있는가? 또 변화하는 과학계의 현실에 대해서 사범교육 속의 실험교육은 어떻게 대응하고 있는지? 이러한 부분에 대해서 함께 고민하고 토의하는 기회를 갖고자 한다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDCOMM-5**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 차정호

과학의 본성에 초점을 둔 과학철학 및 과학사 수업이 예비 화학 교사들의 과학에 대한 인식에 미치는 효과

백성혜

한국교원대 화학교육과

과학 수업을 통해 중등 학생들에게 과학의 본성을 지도하는 것은 과학 교육의 주요 목적 중 하나인 과학적 소양의 함양을 위해 필요하다. 그러나 아직까지 많은 과학교사들과 예비 과학교사들은 과학의 본성을 인식하거나, 이를 지도할 필요성을 인식하지 못하고 있다. 이 연구에서는 예비 화학교사들을 대상으로 과학의 본성에 대한 인식의 유형을 조사하고, 과학의 본성을 직접적으로 다룬 명시적인 수업을 통해 이들의 인식이 변화하는지 알아보았다. 수업 내용에는 다양한 사례와 탐구 실험 등을 통해 과학 지식의 잠정성, 과학 지식의 창안, 관찰과 추론, 관찰의 주관성 등의 내용이 드러나도록 구성하였다. 연구 결과, 과학 지식의 잠정성, 이론의 생성, 실험 목적 등에 대한 예비 교사들의 인식은 후기실증주의 관점으로 변화한 것으로 나타났다. 뿐만 아니라, 과학의 본성에 대한 인식을 통해 과학 교과서에 대한 비판적 안목도 형성되었으며, 과학의 본성을 중등 학생들에게 가르칠 필요가 있음도 인식하였다. 앞으로 예비 과학교사 교육과정에 과학의 본성에 관련된 수업을 포함시킴으로써 이들이 과학 교사로서 학생들을 지도할 때 필요한 능력을 길러줄 필요가 있다. 특히 과학 교사들이 교과서의 내용을 재구성하여 전달할 수 있는 능력을 갖추기 위해서는 과학의 본성에 대한 인식이 필요하다.

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장소: 대구엑스코
발표코드: **EDCOMM-6**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 16:40, 좌장: 차정호

사범대학 화학교육과 학생들의 진로 목표와 대학 생활 계획을 분석하여 살펴본 교사양성대학의 정체성과 사범대학에서 화학교육의 방향성

박종석

경북대 화학교육과

사범대학은 목적대학으로서 우수한 교사양성에 기여해온 바가 크다. 그러나 해마다 임용되는 교사수가 적어지고, 재수 또는 삼수 이상의 시간을 소요하며 임용 시험에 매달리게 되는 현실로 인해 교사양성대학의 정체성은 큰 타격을 받고 있다. 특히 최근 MEET, DEET, PEET 등은 사범대학 화학교육과 학생들의 진로에 큰 영향을 미치고 있다.이에 교사양성대학으로서 사범대학 화학교육과의 정체성을 알아보고자 사범대학에서 화학교육의 방향성을 제언하기 위해 대구시에 소재한 K 대학교 사범대학 화학교육과 학생들을 대상으로 인생 로드맵을 작성 하게 하고, 성별과 학년에 따른 진로 목표와 대학 생활 계획을 분석하였다. 분석 결과 첫째, 성별에 따른 진로목표와 영어공부계획에서 통계적으로 유의미한 차이가 있었는데 여학생들의 의학계 진로목표 비율이 높아 영어공부계획 비율도 높게 나타났다. 둘째, 학년에 따른 영어공부, 여행, 학점관리, 봉사활동, 교환학생 계획에서 차이가 있었는데 사범계 진로목표 비율이 높은 3 학년이 1, 2 학년에 비해 영어공부, 여행, 학점관리, 교환학생을 계획한 비율이 낮았다. 봉사활동을 계획한 비율은 전반적으로 낮았으나 2 학년 복학생들의 비율이 높았다. 셋째, 진로목표에 따른 영어공부계획과 학점관리계획에서 차이가 있었는데 의학계 진로목표 학생들의 비율이 높았다. 이는 사범대학이 목적대학이라는 본래의 특성보다는 현실적인 진로 선택과 생활 계획을 우선하기 때문으로 여겨진다. 따라서 사범대학의 정체성 확립을 위해 재학생들의 진로 지도에 신중을

기할 필요가 있으며, 한편으로 현실을 고려한다면 교사양성대학에서 화학교육의 방향성을 재고할 필요가 있음을 알 수 있다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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장소: 대구엑스코
발표코드: **EDCOMM-7**
발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 금 17:10, 좌장: 차정호

고등학교 과학영재학생들의 국제공동 연구활동

오진호

KAIST 부설 한국과학영재학교

국가별로 미래과학 기술기반 사회에 필요한 창의적인 문제해결력을 지닌 핵심 인재를 양성하기 위한 국가적인 차원에서 다양한 과학영재교육들이 이루어져 오고 있다. 우수한 잠재력을 지닌 과학영재를 조기에 발굴하여 미래 우수한 과학자로 양성하기 위해서는 국가차원에서 지속적인 지원과 더불어서 과학영재교육 프로그램 개발과 우수한 학생들을 지도할 수 영재교육 교사의 양성이 필수적인 요소이다.특히, 미래 창의적인 문제해결력을 지닌 핵심 과학자 양성을 위한 과학영재교육 프로그램들 중에서 '자기주도적인 연구활동'이 중요한 프로그램으로 자리를 잡아가고 있다. 국가차원의 과학영재교육을 지원하고 있는 싱가포르, 미국, 홍콩, 태국, 이스라엘, 러시아 등의 과학영재교육 프로그램에서 고등학교에서부터 학생들이 자신의 관심분야 또는 재능이 있는 분야에서 자기주도적인 연구활동을 관련분야의 과학자 또는 교사들의 사사 지도를 통해 수행하는 프로그램을 운영하고 있다.한국과학영재학교에서도 2 학년 R&E(research & Education)활동을 중심으로 1 학년에서는 창의기초연구와 3 학년 졸업연구 또는 KAIST HRP 프로그램을 통해 자신의 관심분야에서 자기주도적인 연구활동을 수행하도록 하고 있다.본 연구에서는 한국과학영재학교 연구중심프로그램과 한국과학영재학교와 연구중심의 과학영재교육 프로그램을 운영하고 있는 국외영재학교들간의 국제공동 연구활동을 소개한다.또한 고등학교에서부터 과학영재학생들간의 국제공동 연구활동을 통해 학생들이 미래 훌륭한 과학자로 성장하고 또한 국제적인 리더쉽을 키워나갈 수 있는 과학영재교육 프로그램을 제한하고자 한다.

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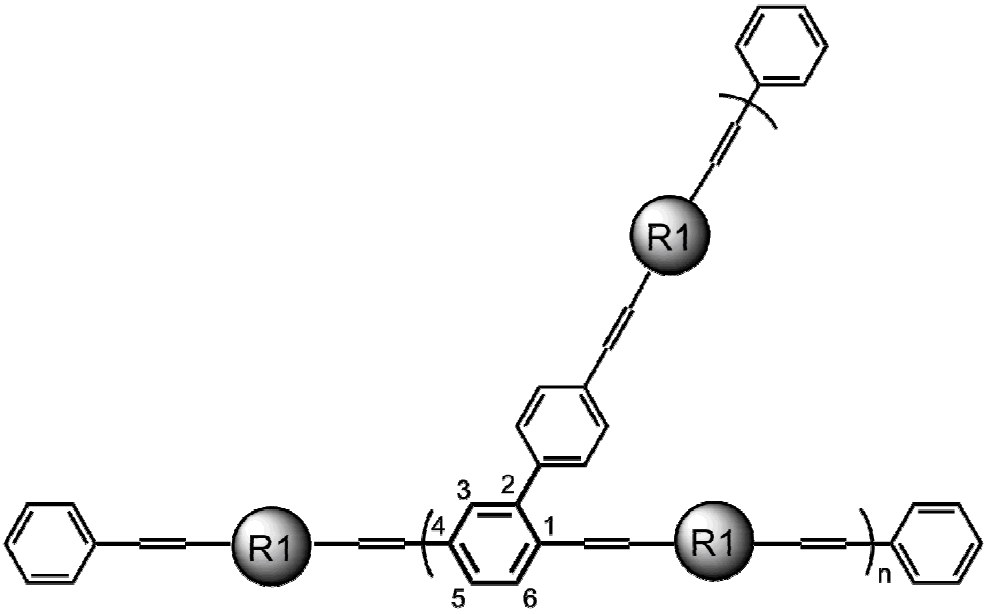
장소: 대구엑스코
발표코드: **POLY.O-1**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 09:50, 좌장: 강영종

Synthesis and Emission Color Tuning of Highly Luminescent π-Conjugated Hyperbranched Polymer

윤원식, 박수영

서울대 재료공학부

π-Conjugated polymeric optoelectronic materials displaying strong absorption and emission properties are drawing great scientific attention. Particularly, the hyperbranched π-conjugated polymers are being actively investigated due to their distinct advantages over conventional linear conjugated ones attributed to their unique dendritic structure. These hyperbranched π-conjugated polymers deserve special attention in the field of photoelectronic devices, with their outstanding processibility as well as their intramolecular energy/charge transfer properties. In this work, we report on the synthesis and properties of a highly soluble 1,2,4- and 1,3,5-linking hyperbranched π-conjugated polymers comprising fluorene, benzene, and thiophene conjugation unit to give different emission spectra.



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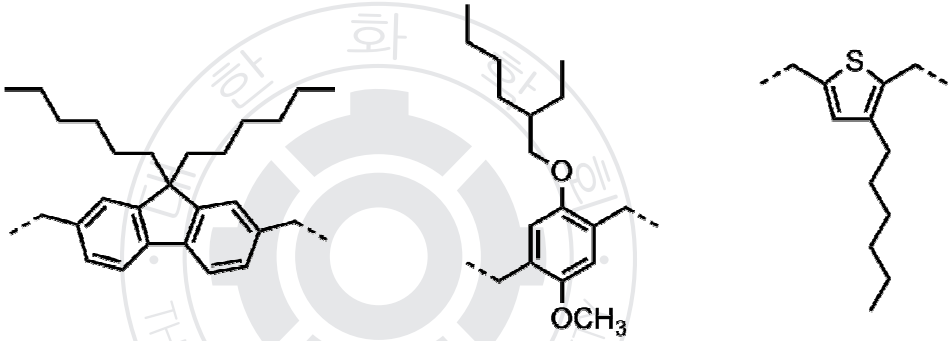

한국화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **POLY.O-2**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 강영종

Realizing 3D metallic and quantum dot patternings by two-photon lithography

Prém Prabhakaran, 장경국, 이광섭

한남대 신소재공학과

Incorporating semiconductor nanocrystals or noble metallic nanoparticles into polymeric microstructures are of much interest due to the potential application of such structures in photonics1. Varying the refractive index within the structures is key to achieving wave guides and photonic crystals. We describe materials and methods aimed at incorporating quantum dots as well as silver into microstructures2. For the former we have synthesized photo-patternable quantum dots and incorporated them into microstructures. For the latter we have followed two approaches first is the direct photoreduction of metallic structures from solutions of metal salts, and the other is the metal coating of fabricated microstructures3-7. Another approach is in-situ generation of noble metal nanoparticles within the microstructure8. We have achieved this with a combination of thermal and ultraviolet UV treatments. This presentation summarizes our work regarding semiconductor nanocrystal and noble metal containing microstructures.

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발표코드: **POLY.O-3**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 강영종

Development of Printable Colorimetric Conjugated Polymer Systems

윤보라, 함대영, *김종만

*한양대 화학공학과 *한양대 응용화공생명공학부*

공액고분자인 폴리다이아세틸렌은 수용액 상에서 합성할 경우 약 640 nm 에서 최대흡수파장을 지니는 청색을 띄다가 외부 환경의 변화에 의해 약 550 nm 에서 최대흡수파장을 지니는 적색의 용액으로 변화된다.본 연구에서는 이러한 폴리다이아세틸렌의 청색에서 적색으로의 색전이 현상을 이용하여 잉크젯 프린터에 잉크로 사용될 수 있는 마이크로에멀젼 시스템과 수용액 시스템을 개발하였다. 폴리다이아세틸렌 마이크로에멀젼은 다이아세틸렌 단량체, 유기용매, 물과 계면활성제로 이루어져있으며, 잉크젯 프린터의 잉크로 적용했을 때 종이, 필름 등과 같은 다양한 기재에 선명한 이미지로 인쇄가 가능하고, 수용액 시스템은 유기용매를 사용하지 않고, 계면활성제를 이용하여 물에 분산되는 다이아세틸렌의 농도를 증가시킴으로써 선명한 이미지를 구현할 수 있다. 또한 인쇄된 이미지를 자외선으로 노광하여 광중합 시킨 후 가열하게 되면 청색에서 적색으로의 색전이 특징을 보이고, 특히 수용액 시스템은 적색으로의 색전이가 일어난 후 다시 청색으로 색이 돌아오는 가역적인 특징을 보이므로, 문서, 지폐, 티켓, 고가의 브랜드 엠블렘 등 다양한 물품의 제조 시 위조방지용 잉크로서 활용될 수 있을 것으로 기대된다.

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장소: 대구엑스코
발표코드: **POLY.O-4**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 정병문

HPLC를 이용한 Complex Polymer의 정밀 분석

안선영, 이효준, 장태현

포항공과대 화학과

Characterization of branched polymers is usually performed by size exclusion chromatography (SEC) separation coupled with light scattering and viscometry detection on the basis of the Zimm-Stockmayer theory. However, SEC cannot do the right job due to its sensitivity on the chain size, not molecular weight and relatively low resolution. Therefore, polymer having different branching numbers and different molecular weight can co-elute. On the other hands, interaction chromatography (IC) is able to separate branched polymers with far better resolution to molecular weight than SEC. By combing more than one chromatographic technique, more detailed information on branched polymers can be obtained. In this work, we attempted to characterize branched polymers by comprehensive two-dimensional liquid chromatography (2DLC) and the two dimensional mappings with respect to the branching numbers and molecular weight are presented.

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장소: 대구엑스코
발표코드: **POLY.O-5**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 정병문

Bio-inspired Surface Immobilization of Polymers on Metal Oxide Nanoparticles for Biomedical Applications

배기현

KAIST 생명과학과

A variety of inorganic nanomaterials such as gold and iron oxide nanocrystals, and quantum dots have drawn significant attention for therapeutic and diagnostic applications. We report herein a bio-inspired approach to surface functionalization of metal oxide nanoparticles with 3,4-dihydroxy-L-phenylalanine (DOPA) conjugated polymers. DOPA is a modified amino acid found within unique adhesive proteins of marine mussels (*Mytilus edulis*), and is known to bind strongly to the surface of diverse metal oxides via metal-oxygen coordination bonds. Taking advantages of strong binding ability of DOPA, we have developed metal oxide nanoparticles stabilized with various natural/synthetic polymers, such as hyaluronic acid, polyethylene glycol (PEG), and polyethylenimine (PEI). These novel nanomaterials could be potentially utilized as multifunctional agents for cancer therapy using therapeutic siRNA and MRI-based diagnosis.

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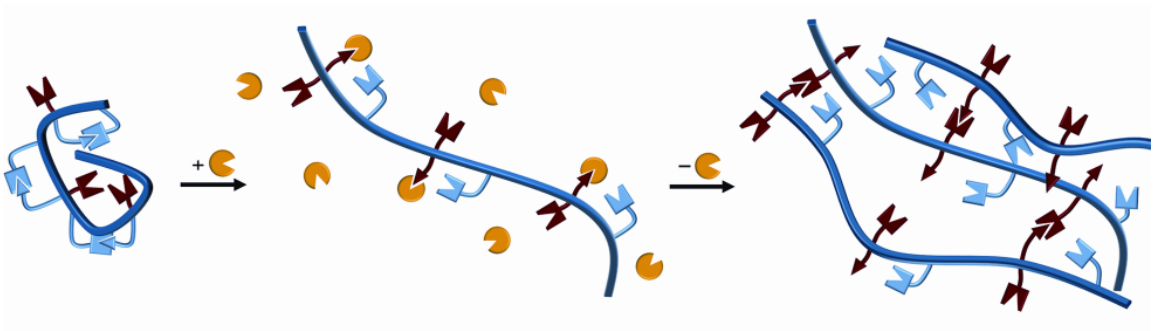
장소: 대구엑스코
발표코드: **POLY.O-6**
발표분야: 신진 고분자 연구자 포럼
발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 정병문

Polymeric Gelator via Hydrogen Bonding Modulation

가두연, 서명은, 김상율

KAIST 화학과

Organogelators are interesting self-assembled materials that can immobilize organic liquids at low concentrations through the formation of self-assembled fibrillar networks. Most organogelators are based on the self-assembly of low-molecular-weight compounds via hydrogen bonds. Consequently, they usually form gels in nonpolar solvents such as benzene or n-hexane, and the resulting physical gels possess poor mechanical properties. Besides the reversible hydrogels based on block copolymers, homopolymeric organogelators relying on specific intermolecular interactions have been rarely studied. Here, we report a novel polymeric gelator based on the poly(arylen ether amide), a high-performance polymer consisting of aromatic rings and amide linkages. By introducing an o-nitroanilide motif into the backbone, unusual gelation behavior in polar aprotic solvents was achieved via solvent-induced intermolecular hydrogen bonding of the o-nitroanilide.



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장소: 대구엑스코
발표코드: **PHYS.O-1**
발표분야: 이론 및 실험 물리 화학 포럼
발표종류: 구두발표, 발표일시: 금 13:30, 좌장: 박준범

Electron Transfer from Axial Ligand to S1- and S2-Excited Tetraphenylporphyrins

조대원, *Tetsuro Majima, *Mamoru Fujitsuka

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Photoinduced processes of a series of phosphorus and Sb-tetraphenylporphyrin (PTPP and SbTPP) derivatives ([PTPP- and SbTPP-$(NHC_6H_4X)_2]^+Cl^-$, X= OCH_3, CH_3, H, Cl, CF_3, and CN) have been investigated by using subpicosecond spectroscopic methods such as fluorescence up-conversion technique. The S2 fluorescence of various SbTPP derivatives was observed for the first time. It was revealed that the S2 fluorescence lifetime changed depending on the donor-ability of the ligand because of the contribution of the charge separation to the S2 excited SbTPP, which was confirmed by transient absorption spectroscopy. On the other hand, the S2 fluorescence lifetime PTPP-OH_2 was estimated to be 1.5 ps. Both S2 and S1 fluorescence bands of PTPP-$(NHC_6H_4X)_2$ were difficult to observe, indicating the existence of an additional deactivation process such as charge separation (CS). From MO calculation and cyclic voltammetry, PTPP and the axial ligand are expected to act as an acceptor and a donor, respectively, upon excitation of PTPP. The CS via S2 state was confirmed by the femtosecond transient absorption of radical anion of PTPP. Furthermore, The CS via S1 state of PTPP was also observed. The CS rate via S1 state was faster than that from the S2 state. The free energy dependence of the electron-transfer rates was discussed on the basis of Marcus theory.

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Multiscale simulations of nanoparticles, polymers, and membranes for drug delivery

Hwankyu Lee

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Interactions of nanoparticles, polymers, and membranes have been studied using all-atom andcoarse-grained molecular dynamics simulations. The following topics will be presented: (1)membrane curvature and pore formation induced by differently sized, charged, shaped, andconcentrated nanoparticle (dendrimer) and linear polymer; (2) conformation and hydrodynamicsof polyethylene glycol (PEG) in water and on surfaces; (3) self-assembly and phase behavior ofPEG-conjugated vesicles, bicelles, and micelles; (4) parameterization of all-atom and coarsegrainedmodels for simulations described above. This work aids in the rational design ofnanoparticles and drug complexes for drug delivery, and development of accurate nanopores forbiosensor applications.

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방사성 핵종을 이용한 새로운 광학영상 기법

박정찬, *안광일, **하영수, **왕은경, ***김정영, 유정수

*경북대 의과대학 분자의학교실 *한국원자력의학원 방사성의약품 개발실 **경북대 의과학과 ***한국원자력의학원 방사성의약품연구팀*

핵의학과 광학 영상은 여러 가지 면에서 상호보완적이므로 동위원소를 사용하여 광학 영상을 얻거나 핵의학/광학 이중 영상을 하나의 영상 프로브로 얻을 수 있다면 많은 장점들이 있을 것이다. 서로 다른 두 종류의 방사성 핵종을 생쥐에 주사한 후 발광 영상을 측정하였다. 다른 붕괴모드를 가지는 다양한 방사성 핵종의 발광 세기는 발광 영상과 체외 발광측정기를 사용하여 측정하였다. 방사성 요오드 표지된 허셉틴은 생쥐를 이용한 종양모델에 주사하였고 발광 영상을 획득하였다. [^{32}P]인산염 용액에 담겨진 식물도 발광 모드에서 촬영하였다. 양자점이 첨가되기 전과 후의 ^{124}I 용액의 빛 세기 변화를 모니터하였다. Radio-TLC 판은 발광 영상 모드에서 영상을 획득하였다. 발광 영상은 주사된 방사성 추적자의 예상 분포 양상과 일치하였다. 고 에너지 입자를 방출하는 방사성 핵종들은 강한 발광 신호를 보여주었다. NIH3T6.7 암세포는 방사성 요오드로 표지된 허셉틴에 의해 광학과 핵의학 영상 모두에서 분명하게 관찰되었다. 식물에서의 [^{32}P]인산염 섭취는 발광 영상에 의해 쉽게 추적 가능하였다. ^{124}I 용액에 양자점의 첨가로 발광 신호가 상당히 증가하였다. 발광 영상으로부터 계산된 방사화학적 순도는 radio-TLC 스캐너와 좋은 상관 관계를 보여 주었다. 붕괴하는 동안 고 에너지 β^+ 또는 β^- 입자를 방출하는 많은 방사성 핵종들은 주로 체렌코프 복사에 의해 발광 모드에서 광학영상을 얻을 수 있음을 발견하였다. 체렌코프 영상은 광학과 핵의학 영상 사이에서 매우 귀중한 교량과 새로운 광학 영상 플랫폼을 제공해 줄 것으로 여겨진다.

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TAMING MOLECULAR BEAMS; TOWARD A MOLECULAR LABORATORY ON A CHIP

Samuel Meek, G. Santambrogio, M. Abel, H. Conrad, *B.G. Sartakov, G. Meijer

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Getting ever better control over gas-phase molecules is an important research theme and drives progress in the field of molecular physics. The motion of neutral molecules in a beam can be manipulated with inhomogeneous electric and magnetic fields. Static fields can be used to deflect or focus polar molecules, whereas time-varying fields can be used to decelerate or accelerate beams of molecules to any desired velocity. This molecular beam technology offers possibilities ranging from ultrahigh-resolution spectroscopy and novel scattering experiments to lifetime measurements on trapped molecules [1].I will report in particular on our recent experiments demonstrating trapping of metastable carbon monoxide molecules on a chip [2] using direct loading from a supersonic beam [3,4]. Upon arrival above the chip, the molecules are confined in tubular electric field traps of about 20 micrometer diameter, centered 25 micrometer above the chip, that move along with the molecular beam at a velocity of several hundred meters per second. These moving traps and the molecules they contain can be brought to a complete standstill over a distance of only a few centimeters. After a certain holding time, the molecules can be accelerated off the chip again for detection. This loading and detection methodology is applicable to a wide variety of polar molecules, and enables the creation of a molecular laboratory on a chip.Non-adiabatic transitions to untrappable states present a critical loss channel from the microtraps. While these losses can be suppressed by using the ^{13}CO isotopologue, more recent experiments have demonstrated the suppression of losses in ^{12}CO by applying a homogeneous magnetic field to split the low field seeking states from those unaffected by the electric fields. By tuning the strength of the magnetic field, the minimum splitting needed to prevent all losses can be quantitatively understood.References[1] S.Y.T. van de Meerakker, H.L. Bethlem, and G. Meijer, Nature Physics 4, (2008) 595.[2] S.A. Meek, H. Conrad, and

G. Meijer, Science 324, (2009) 1699.[3] S.A. Meek, H.L. Bethlem, H. Conrad, and G. Meijer, Phys. Rev. Lett. 100, (2008) 153003.[4] S.A. Meek, H. Conrad, and G. Meijer, New J. Phys. 11, (2009) 055024.[5] M. Kirste, B.G. Sartakov, M. Schnell, and G. Meijer, Phys. Rev. A 79, (2009) 051401(R).

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THE KOREAN CHEMICAL SOCIETY

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Quantum reflection of He_2 and He_3 from a plane ruled grating

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The feeble long-range van der Waals attraction between two ground-state helium atoms is barely strong enough to support a bound-state dimer. Its tiny dissociation energy of 10^{-7}eV comes along with a large mean internuclear separation of more than 5 nm. Helium trimer also has very small dissociation energy of 10^{-5}eV. In this work we demonstrate that He_2 and He_3, despite their fragility, can scatter non-destructively from a solid surface. The ambiguity in their mass spectrometric detection is discarded by diffraction from a plane ruled grating. The observation is attributed to 'quantum reflection', a matter-wave phenomenon that leads to reflection of the dimer and trimer many nanometers above the surface, where the surface induced forces are sufficiently weak to not dissociate them.

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Gaint Stark Effect in Double-stranded Porphyrin Ladder Polymers

강홍석, *Anup Pramanik

*전주대 나노신소재공학과 *전주대 공학연구소*

Using the first-principle calculation, we have investigated the binding energy and electronic structure of double-stranded Zinc porphyrin ladder polymer recently synthesized. First, we find that there is an appreciable degree of binding between the porphyrin strands and dipyridyl (DPY) bridging unit in the ladder. Secondly, electronic structure calculation shows that the polymer is a semiconductor with a direct gap at the zone boundary, which is originated from the fact that the valence and conduction band are derived from the HOMO and LUMO of the underlying porphyrin molecule. Most importantly, application of electric field along the direction perpendicular to the porphyrin units significantly reduces the band gap, ultimately converting the ladder polymer to a metal at the field strength of 0.1V/A. Under electric field, hole conduction and electronic conduction occurs entirely through each of the two porphyrin units, rendering it useful in nanoelectronics. Finally, we will also discuss the effect of different metal ions and terminal atoms on the stability and electronic structure of the ladder polymer.

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Multiparameter single-molecule fluorescence microscopy of macromolecules

김학준, *Carl C. Hayden

*덕성여대 화학과 *Sandia National Laboratories*

Conformational changes of macromolecules such as protein, DNA, RNA in solutions are the key to understanding biological functions of living body. Fluorescent dye molecules attached to the site of interest are used to report the local chemical environment change correlated to the conformational change of macromolecules. We have carried out experiments using a custom-built multiparameter fluorescence microscope that measures the wavelength, emission delay relative to excitation (excited-state lifetime), and chronological time (intensity) for each detected photon. The simultaneous measurement of multiple fluorescence features allows us to assign event with high confidence in low signal-to-background conditions. We have investigated a single-molecule study of a TMR-biocytin bound to streptavidin immobilized on PEG-biotin surfaces as well as that encapsulated in a surface tethered vesicle to understand the interaction between a single dye molecule and a single protein. Our preliminary results show that the single-molecule study of a TMR-biocytin bound to streptavidin encapsulated in a surface-tethered vesicle agrees well that of bulk measurements.

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‘Smart’ Gold Nanoparticle Conjugates for Combined Photothermal and Chemo-Therapy of Cancer Cells

남주택, 원나연, 김성지

포항공과대 화학과

Noble metal nanostructures can be ideal candidates for photothermal cancer therapy by their large light extinctions at surface plasmon resonances and the efficient heat conversions. We developed a new photothermal therapy concept using ‘smart’ gold nanoparticle that exploit coupled surface plasmon modes of nanoparticle aggregates. ‘Smart’ gold nanoparticles are designed to form aggregates under mild acidic conditions such as in intracellular environment. With the relatively small size of 10 nm, ‘smart’ gold nanoparticles can be efficiently internalized into cancerous cells. Triggered by the pH change, the nanoparticles rapidly form aggregates inside cells, and the aggregates accumulate as the exocytosis is blocked by the increased size. The pH-induced aggregation of gold nanoparticles shifts the absorption to far-red and near-infrared. This shift was successively utilized for selective and deep tissue penetrating photothermal therapy. We also developed ‘smart’ gold nanoparticle conjugates where molecular cancer drugs such as doxorubicins were covalently conjugated to the ‘smart’ gold nanoparticles. This ‘smart’ gold nanoparticle conjugate acts as a drug delivery vehicle as well as a sensitizer for photothermal therapy. When triggered by the intracellular environment, ‘smart’ gold nanoparticle conjugates can form gold nanoparticle aggregates and simultaneously can release the loaded cancer drugs, allowing localized, region-specific delivery of both photo-sensitizer and cancer drugs inside the cancer cells. Combination of photothermal and chemo-therapy shows significantly improved therapeutic efficacy of maximally over 6 folds compared to the projected sum of two treatments alone, suggesting huge synergistic effect between two modalities.

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Addition of Diphenyl Phosphate to Alkynes Catalyzed by Gold

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*강원대 화학과 *KAIST 화학과*

Conversion of carbonyl compounds into enol phophates is of a great synthetic importance since enol phosphates are versatile intermediates which undergo various synthetically useful transformations. The major issue in this transformation is selectivity . Especially, the more substituted thermodynamic enol derivatives from unsymmetrical ketones normally predominate under thermodynamic conditions but to not form exclusively, which is a serious problem in organic synthesis. Thus, the preparation of thermodynamic enol phosphates as highly pure form is of synthetic importance and still a very challenging problem. We have developed the hydrophophoryloxylation reaction of alkynes using diphenyl phosphate in the presence of $Ph_3PAuCl/AgPF_6$ to afford the kinetic enol phophates. Whereas the reaction using $(C_6F_5)_3PAuCl/AgOTf$ gave the thermodynamic enol phosphates as highly pure forms. In addtion, $(C_6F_5)_3PAuOTf$ proved to be highly efficient catalyst for the isomerization of kinetic enol phosphates into thermodynamic isomers.

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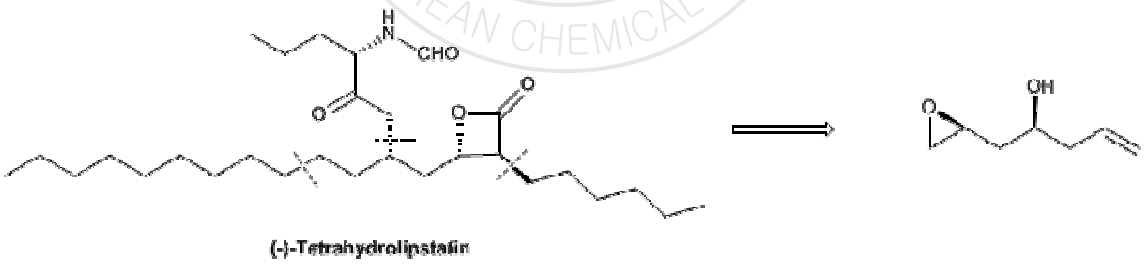
Synthetic Studies of (-)-Tetrahydrolipstatin

최경환, 김혜미, 태진성

연세대 화학과

(-)-Tetrahydrolipstatin(THL) is an anti-obesity drug marketed under tradename of Xenical or Orlistat internationally. THL is a saturated derivative of natural product lipstatin isolated from Streptomyces toxytricini in 1987 and has a β-lactone moiety that can react with pancreatic lipase enzyme. We have tried to synthesize (-)-THL from an enantioenriched (*S,S*)-epoxy alcohol generated by hydrolytic kinetic resolutions(HKR) method using Jacobson's catalyst. From the (*S,S*)-epoxy alcohol, β-lactone structure was established via epoxide ring opening and lactonization strategy. We expected that saturated-carbon chain of (-)-tetrahydrolipstatin could be achieved by enantioselective α-alkylation and cross metathesis



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Phosphoinositide 3-Kinase Inhibitors that double as Intracellular Fluorescent Probes

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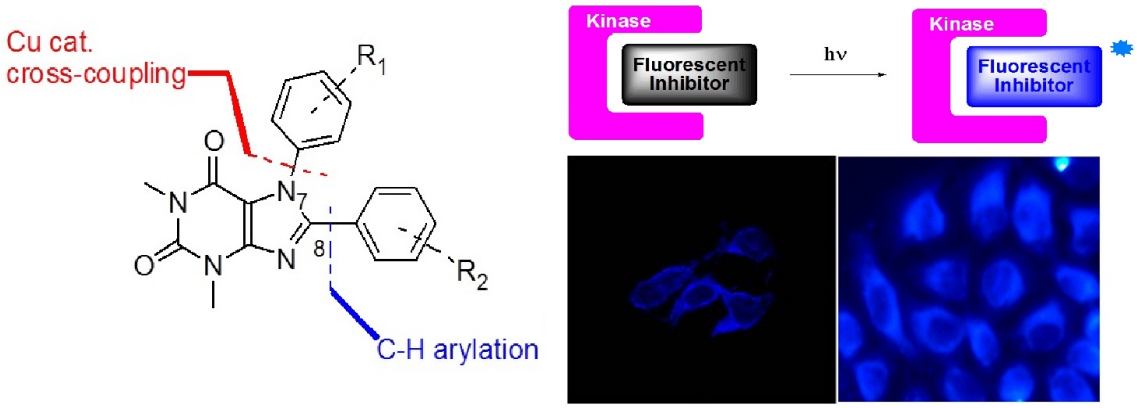
An understanding of the intracellular drug distribution and fate in biological system is invaluable, since it can provide information whether drug reaches its desired target and a biological rationale for the design of new therapeutics with improved properties.An efficient and versatile synthetic approach for the preparation of highly substituted xanthine derivatives has been developed by a combination of direct N7- and C8-arylation. The xanthine core is structurally similar to ATP to fit into ATP binding site, while H-bonding of R1 and R2 moiety with S774 and K802 can increase binding affinity. This xanthine core skeleton can accommodate various emission maxima and quantum yield simply by changing substituents at the R1 and R2 positions, having different electronic properties. Herein, we report cell-permeable fluorescent PI3K inhibitors in which some part of the fluorophores were engineered to be pharmacophores binding to PI3K, and describe the monitoring of their distribution in cells.



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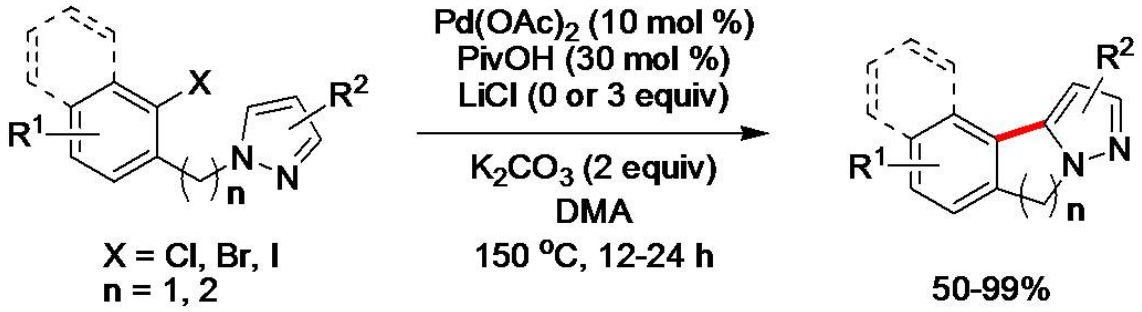
Palladium-Catalyzed Intramolecular C-H Bond Activation of Pyrazoles

최영록, *허정녕

*고려대 화학과 *한국화학연구원 신약연구단*

One of the most attractive methods for forming C-C bonds with a catalytic system is through C-H bond functionalization. Transition-metal catalyzed transformations represent a central strategy in this respect, and in particular Pd catalyzed reactions play a pivotal role. In connection with our ongoing studies in the synthesis of biologically important heterocyclic compounds, which possess a pyrazole motif, we became interested in exploring the intramolecular C-H bond activation of pyrazole scaffolds. Although elegant approaches of C-H bond activation of pyrazoles have been developed, intramolecular C-H bond activation of pyrazole motifs is somewhat limited. Herein, we have established a novel, direct, onestep synthesis of pyrazolo[5,1-*a*]isoindoles via Pd-catalyzed intramolecular C-H bond activation. The use of LiCl was found to be essential in these reactions, to suppress further C-H bond activation at the C3 position of pyrazolo[5,1-*a*]isoindole when the pyrazole is unsubstituted. Furthermore, we have applied this protocol to the synthesis of pyrazolo[5,1-*a*]isoquinolines possessing a six-membered central ring system. Fully substituted pyrazolo[5,1-*a*]isoindole was also synthesized by using sequential intra- and intermolecular C-H bond activation



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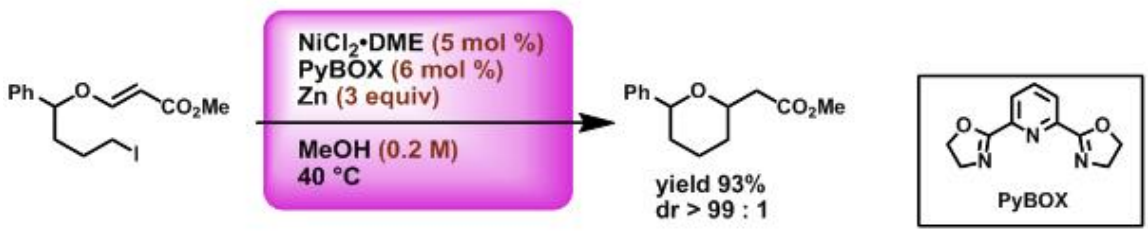
Nickel-catalyzed cyclization of haloalkenes: a tin-free radical reaction

김혜진, 이철범

서울대 화학부

Free radical mediated reactions have emerged as powerful tools in synthetic organic chemistry. Radical cyclizations using organotin hydrides are among the most common methods for constructing cyclic structures from simple alkenyl halides. However, the high toxicity of the tin reagent and the difficulty of removing it from the reaction products have been significant shortcomings. Among the efforts for development of tin-free processes, the transition metal promoted radical reactions offer a useful alternative to stannane and other main group metal based processes. We developed a nickel-catalyzed cyclization of haloalkenes as a new method for tin-free radical reactions. This method is operationally simple and applicable to the cyclization of alkyl halides with a variety of acceptors including vinyl sulfones and vinyl sulfoxides, and even unactivated olefins. The new protocol presented here gives functionalized carbo-, oxa-, and azacycles under very mild conditions with high yields.



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Dicyanovinyl Substituted Oligopyrrolic Macrocycles as Models for Cyanide-Selective Ratiometric Chemosensors

이창희, 홍성진

강원대 화학과

Oligopyrrolic macrocycles such as calix[4]pyrroles and strapped calix[4]pyrroles which are originally transparent in visible region, becomes yellow colored (λmax =403 nm in acetonitrile) by introduction of dicyanovinyl or nitrovinyl group at beta-pyrrolic position. These macrocyclic compounds form stable host-guest complexes with most of anions through hydrogen bonding with hypsochromic shift of the absorption spectra. However, when the hosts are titrated with cyanide anion, complete bleaching of the colour is observed. The experimental evidences clearly indicate that the cyanide is added to the alpha-position of dicyanovinyl group forming a ketimine. These dual functional, chemodosimeteric sensors show high selectivity toward cyanide anion. Association contants were measured and the values are compared with those of other calix[4]pyrroles. The current receptors that bear both anion binding site and nucleophile-selective electrophilic site could be beneficial achieving higher anion selectivity and reducing inhibitory effect of other anions.

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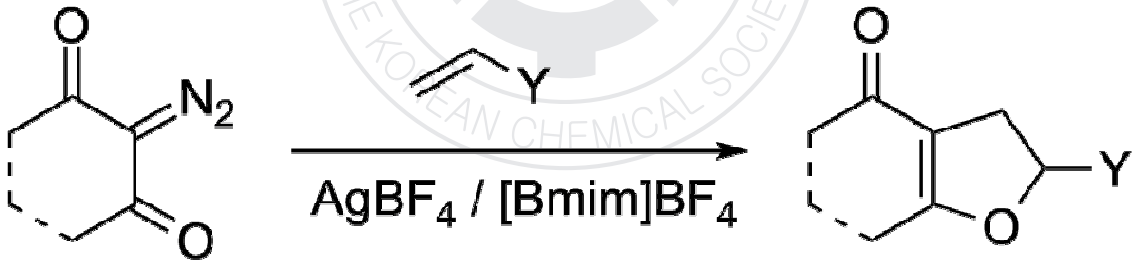
발표종류: 구두발표, 발표일시: 금 09:47, 좌장: 홍승우

Efficient Synthesis of 2,3-Dihydrofurans by $AgBF_4$/[Bmim]BF_4-Catalyzed [3+2] Cycloaddition of Cyclic Diazodicarbonyl Compounds with Olefins

하립개, 이용록

영남대 화학공학부

A novel and efficient method for the synthesis of 2,3-dihydrofurans was achieved by the reaction of cyclic diazodicarbonyl compounds with styrene and vinyl acetate. The key strategy was $AgBF_4$/[Bmim]BF_4-catalyzed [3+2] cycloaddition reactions.



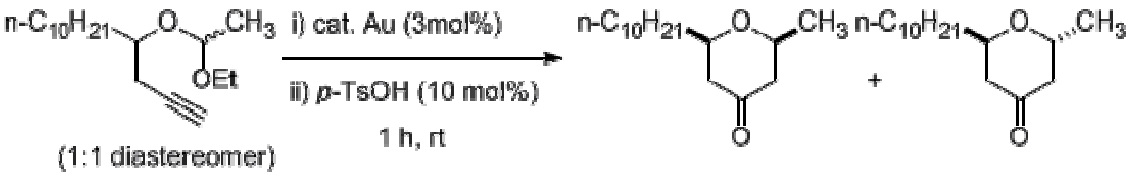
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.O-8**
발표분야: 대학원생 구두발표
발표종류: 구두발표, 발표일시: 금 09:55, 좌장: 홍승우

Gold(I)-Catalyzed Cycloisomerization of O,O-Acetals Generated from Homopropargylic Alcohols to Highly Substituted Tetrahydropyran-4-ones

배효진, 이영호

포항공과대 화학과

Recently, we have developed a new method for the synthesis of highly substitutued cis-2,6-tetrahydropyranones through gold(I)-catalyzed cycloisomerization of 4-(alkoxyalkyl)oxy-1-ynes as key event, which features catalytic model of Petasis-Ferrier rearrangement.1 In this cycloisomerization, it is noteworthy that diastereoselectivity of highly substitutued 2,6-tetrahydropyranones is significantly affected by ligand effect of cationic (tri-alkylphosphine) gold complexes. The synthetic utility of this method is expanded by dihydroxylation of cycloisomerized intermediate, enol ether, to 3-hydroxy-2,6-tetrahydropyran-4-one as a single diastereomer.



cat.	yield		
$Au[P(C_6F_5)_3]^+SbF_6^-$	57%	:	28%
$Au[P(C_6H_5)_3]^+SbF_6^-$	63%		13%
$Au[P(t\text{-}Bu)_2(o\text{-}Ph)Ph](CH_3CN)^+SbF_6^-$	72%	:	9%

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발표종류: 구두발표, 발표일시: 금 10:02, 좌장: 홍승우

Pd-Catalyzed ortho-Olefination of Acetanilides: Mechanistic Studies and Kinetic Isotope Effect

김병석, 윤소원

한양대 화학과

Recently, we have developed a Pd-catalyzed ortho-olefination of acetanilides under mild conditions with broad substrate scope. To gain insight into this reaction, mechanistic studies were extensively carried out. The preparation and characterization of potential intermediates such as palladacycle were achieved and the subsequent reaction with methyl acrylate underwent smoothly to give the corresponding ortho-olefinated acetanilide. Palladacycle could also catalyze the oxidative coupling of acetanilide with methyl acrylate to afford the corresponding ortho-olefinated acetanilide in good yield. Furthermore, kinetic isotope experiments suggest that cleavage of the C-H bond at the ortho position is involved in the rate-determining step.

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발표분야: 대학원생 구두발표

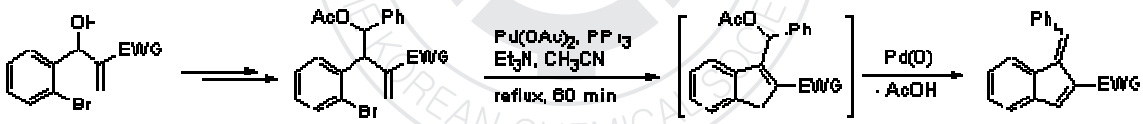
발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 홍승우

Facile synthesis of benzofulvene derivatives from Baylis-Hillman adducts: In-mediated Barbier reaction combined with Pd(0)-catalyzed intramolecular Heck-elimination cascade

김고훈, 박보람, 김재녕

전남대 화학과

A facile synthesis of benzofulvene derivatives was carried out starting from the Baylis-Hillman adducts of 2-bromobenzaldehyde *via* the sequential bromination, In-mediated Barbier reaction with aldehyde, acetylation, Pd-catalyzed intramolecular Heck reaction, and the elimination of AcOH.



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발표코드: **ORGN.O-11**
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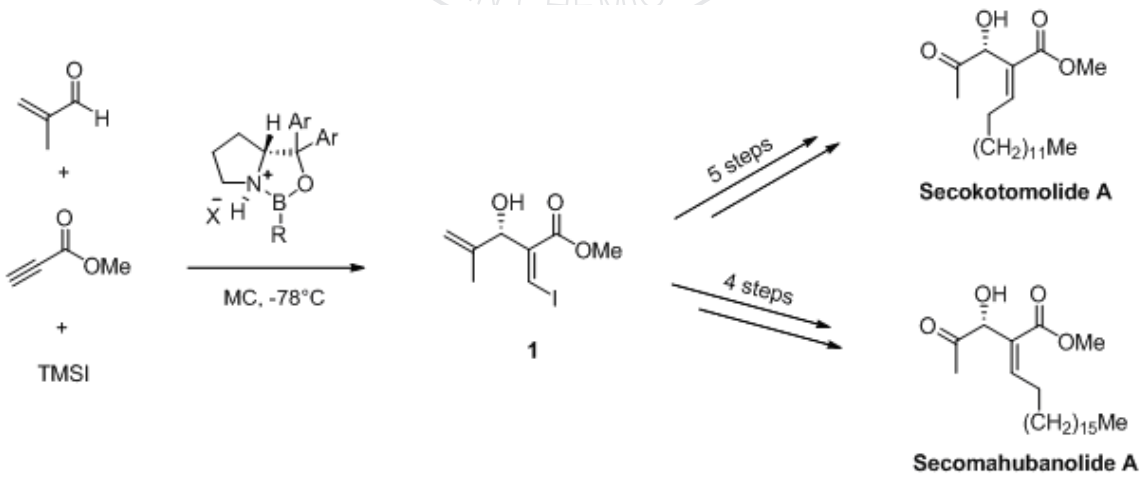
발표종류: 구두발표, 발표일시: 금 10:17, 좌장: 홍승우

Total Synthesis of Secokotomolide A and Secomahubanolide A

문순영, 류도현

성균관대 화학과

Secokotomolide A and Secomahubanolide A were isolated from *cinnamoum ketones* and *machilus zuihoensis* respectively. Secokotomolide A was found to induce significant cell death in the human HeLa cell line by apoptotic-realted DNA damage. Secomahubanolide A shows marginal cytotoxicity against NUGC and HONE-1 cancer cell lines.The enantioselective synthesis of Secokotomolide A and Secomahubanolide A, has been accomplished from the readily available chiral (Z)-β-iodo Morita-Baylis-Hillman ester (1) as a key intermediate. Asymmetric three component coupling reaction furnished (Z)-β-iodo MBH ester (1) in high enantioselectivity. Additional few steps afforded both natural products in high overall yield.



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장소: 대구엑스코
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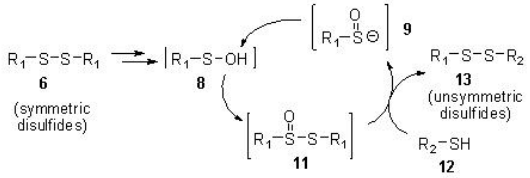
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 강은주

A Traceless, One-pot Preparation of Unsymmetric Disulfides from Symmetric Disulfides through a Repeated Process of Sulfenic Acid and Thiosulfinate Intermediates

한민수

고려대 화학과

Disulfides are found in numerous natural products and biologically significant functional materials. Numerous disulfides occur naturally, and the study of their biogenesis should lead to fascinating results. Although symmetric disulfides can be prepared by the direct transformation of thiols, through treatment with hydrogen peroxide, iodine, chromates, bromine, or sulfuryl chloride, efficient synthetic methods, for unsymmetric disulfides are still in need. Here, we report a simple and convenient preparation of unsymmetric disulfides under mild reaction conditions and in high yields from symmetric disufides through thiosulfinate intermediates. In addition, an important advance in this new methodology is the traceless preparation of unsymmetric disulfides in a one-pot reaction



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발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 강은주

Studies toward the Total Synthesis of Arenicolide A

이정열, 이광국, 이덕형

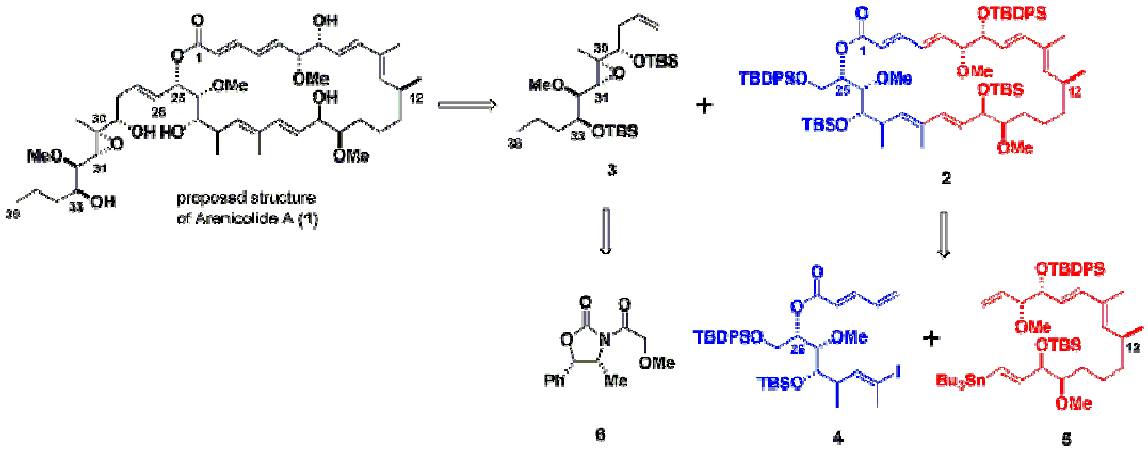
서강대 화학과

Arenicolide A is a 26-membered macrolide with three conjugated dienes and nine chiral centers in the ring. There is one side chain which comprises the C26~C36 carbon chain with five consecutive chiral centers.[1] Effective stereocontrolled syntheses of subtargets C27~C36 3, vinyl iodide 4 and vinyl stannane 5 have been achieved. The synthesis of C27~C36 3 was achieved in 10 steps via anti-epoxidation of α–methoxy allylic alcohol.[2] The stereoselective synthesis of vinyl iodide 4 was performed in 17 steps using methyl (R)-(-)-3-hydroxyisobutrate as a starting material. Vinyl stannane 5 was completed by Wittig reaction and stille coupling of the corresponding fragments as key steps.

References

1. Williams, P. G.; Miller, E. D.; Asolkar, R. N.; Jesen, R. R.; Fenical, W. *J. Org. Chem.* 2007, 72, 5025-5034

2. Lee, J. L.; Han, S. J.; Lee, D. H. *Bull. Korean Chem. Soc.* 2009, 30, 14



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발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 강은주

Platinum-Catalyzed Intramolecular Hydroarylation of Allenyl Arenes: Efficient Synthesis of 1,4-Dihydronaphthalenes

모준태, 이필호

강원대 화학과

Development of an efficient cyclization method is very important for the biological and pharmaceutical applications. During the studies on the addition of allenoate to aryl substrates, we found an interesting intramolecular cyclization reaction. So, we have prepared various allenoates and their cyclization was achieved with platinum. Various type of allenoates applied to the preparation of dihydronapthalene derivatives with this catalytic system. These processes are not only efficiency but also many advantages.

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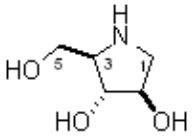
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 강은주

An Efficient synthesis of 5-membered iminosugars and (−)-Swainsonine from Chiral Aziridines

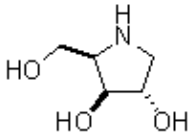
최환근, *심태보, 이원구

*서강대 화학과 *KIST 생체과학연구본부*

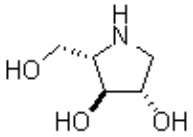
1,4-dideoxy-1,4-imino-D-arabinitol and (−)-swainsonine were turned out to be a potent glycogen phophorylase inhibitor. The glucosidase inhibitors have aroused much interest on account of the possibility that these could be therapeutic agents for treating several diseases such as diabetes, viral infection, cancer and genetic disorder. The oncogene activation triggered the aberrant glycosylation due to an altered cascade expression of glycosyltransferases. It was also turned out that the level of glycosidases was elevated in many cancer patients. The broad spectrum of biological activity, especially anti-cancer activity, of α-glucosidase inhibitors led us to be interested in synthesizing stereoselectively 1,4-dideoxy-1,4-imino-D-arabinitol including its analogues and (−)-Swainsonine. An efficient and facial synthetic approach for the synthesis of 1,4-dideoxy-1,4-imino-D-arabinitol and its analogues was successfully achieved starting from commercially available chiral aziridines. In addition, an efficient synthesis of enantiomerically pure (−)-swainsonine was successfully accomplished using intramolecular cyclization of the amino alcohol which was derived from a readily available 1-(R)-α-methylbenzylaziridine-2-carboxylic acid (−)-menthol ester.



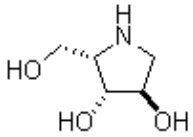
D-AB1 , **1**
(2*R*, 3*R*, 4*R*)



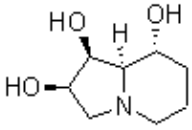
D-DIX , **2**
(2*S*, 3*S*, 4*R*)



L-AB1 , **3**
(2*S*, 3*S*, 4*S*)



L-DIX, **4**
(2*R*, 3*R*, 4*S*)



(-)-swainsonine

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발표분야: 재료화학분야의 최신 연구동향
발표종류: 구두발표, 발표일시: 금 14:00, 좌장: 이기라

Fluoride sensing by catechol-based π-electron systems

안병관, *Xing Wang, *Paul L. Burn, *Paul Meredith

*가톨릭대 *Centre for Organic Photonics & Electronics, The University of Queensland, Queensland, 4072, Australia*

Fluoride plays an important role in a broad range of biological, chemical and medical processes. On the one hand there is positive support for fluoride because of its use in applications such as dental care by fluoridation of drinking water, food additives, and osteoporosis treatment. However, fluoride has been linked to health problems when above the safe concentration limits, and it is also found in chemical and nuclear warfare agents. Real world fluoride detection of fluoride in aqueous solution is difficult as it forms strong hydrogen bonds with water. In this work we have developed new catechol-based sensors that can detect fluoride ions via fluorescence or optical absorption even in the presence of other halides. The level and sensitivity of detection of the sensing molecules is dependent on the chromophore length, which is controlled by the number of thiophene units (one to three) within the chromophore. The sensor with three thiophene units, (E)-2-(2,2'-terthiophen-5-yl)-3-(3,4-dihydroxyphenyl)acrylonitrile, gave the best response to fluoride. By using fluorescence measurements fluoride was detectable over the concentration range 1.7 μM to 200 μM. Importantly, when adsorbed onto a solid support the fluorescent catechol dye could be used to detect the presence of fluoride in aqueous solution.

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발표종류: 구두발표, 발표일시: 금 14:25, 좌장: 이기라

Nanostructured bulk Thermoelectric Materials for Energy Harvesting Applications

한미경, *김성진

*이화여대 화학나노과학부 *이화여대 화학과*

Upon confronting the global warming problem, the global need for utilizing exhausted waste heat has been accelerated. Thermoelectric materials are gathering a great interest as a potential alternative energy source because of their capability of generating electric power using waste heat from, e.g., automobiles. The performance of a thermoelectric material is assessed with the figure of merit ZT defined as $(S^2\sigma/k)T$; where S is the Seebeck coefficient (or thermopower), σ electrical conductivity, κ thermal conductivity, and T is the temperature. To be competitive with conventional refrigerators and generators, one must develop materials with ZT > 3. Bulk-bismuth telluride (Bi_2Te_3) and its alloys are the best room-temperature thermoelectric material found to date. Different approaches have been tried in order to enhance the thermoelectric properties of Bi_2Te_3. Doping is a commonly used way to improve the thermoelectric properties of Bi_2Te_3-based materials. Here, we investigated the effects of Cu doping on the thermoelectric properties of Bi_2Te_3. Cu-doped n-type Bi_2Te_3 was prepared by rapidly cooling the bulk material. Detailed charge transport data including electrical conductivity, Seebeck coefficient, Hall coefficient and thermal conductivity are presented. The addition of Cu results in the changing their physical properties, as well as conduction type. Compared to undoped Bi_2Te_3 the power factor of Cu-doped is substantially increased up to ~38 $\mu W/cm \cdot K^2$. High resolution TEM images of both samples reveal that all systems contain compositional fluctuations at the nanoscopic level and are nanostructured. Inserting additional Cu is very effective in improving electrical conductivity and Seebeck coefficient, and suppressing thermal conductivity, thus enhancing ZT.

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발표종류: 구두발표, 발표일시: 금 14:50, 좌장: 이기라

CdSe Quantum Dot/Fullerene Nanocomposite for Improved Solar Energy Conversion

방진호, *Prashant V. Kamat

*한양대 응용화학과 *University of Notre Dame*

Colloidal CdSe Quantum Dots (QDs) are coupled with thiol-functionalized fullerene (C60) to facilitate the separation of charge carriers. Electron transfer from excited CdSe QD to C60 is monitored by steady-state and time-resolved fluorescence spectroscopy. In this study, ultrafast transient absorption spectroscopy is used to elucidate QD size-dependent electron transfer rate. The spectroscopic analysis reveals that when CdSe QDs are coupled with C60, smaller CdSe QDs show faster electron transfer rate than larger ones, which is consistent with theoretical prediction based on Marcus theory. The newly developed, novel nanocomposite is deposited onto optically transparent electrode via electrophoretic deposition technique, and the photoelectrochemical property of photoelectrodes is evaluated. The photoelectrode, which consists of CdSe QDs/C60 nanocomposite, shows much improved solar energy conversion efficiency than the photoelectrode fabricated with CdSe QDs alone. Despite faster electron transfer process in small-sized CdSe QDs, the photoelectrode with smaller QDs/C60 is less efficient in solar energy conversion than that with larger QDs/C60. This is closely related to size-dependent absorption coefficient of CdSe QDs.

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발표분야: 재료화학분야의 최신 연구동향
발표종류: 구두발표, 발표일시: 금 15:25, 좌장: 방진호

Platinum nanoparticles encapsulated by aminopeptidase: a multifunctional bioinorganic nanohybrid catalyst

김경규

성균관대 의학과

Biomineralization using protein shells is being intensely investigated for the synthesis of inorganic nanomaterials which can be applied to a variety of uses including electronic devices, hydrogen production, and MRI contrast medium. Although huge efforts have been made to expand the application repertoire of protein-shelled nanomaterials, most applications are still limited to their metallic property. We demonstrated that platinum nanoparticles encapsulated by PepA, a bacterial aminopeptidase, can function as a bioinorganic nanohybrid catalyst that can successfully couple platinum-catalyzed hydrogenation and peptidase-catalyzed hydrolysis with biocompatibility. The synthesis of ultra small platinum particles which showed the highest catalytic activity was precisely controlled inside the PepA protein shell to subnanometer scales. Collectively, our findings provide a foundation for the construction of nanobiofactories to produce complex molecules and may be applied to in vivo syntheses of therapeutic molecules or metabolic modifiers.

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발표분야: 재료화학분야의 최신 연구동향
발표종류: 구두발표, 발표일시: 금 15:50, 좌장: 방진호

Properties of supercapacitors made of aligned carbon nanotubes directly synthesized on carbon papers

김웅

고려대 신소재공학부

We demonstrate that vertically aligned carbon nanotubes can be synthesized directly on conductive carbon papers and used as excellent electrochemical capacitors. The carbon nanotubes were synthesized using an Al/Fe catalyst via water-assisted chemical vapor deposition. They grew as fast as ~ 100 um/min and approximately 70% of them had double walls with average diameter of ~ 6 nm. Interestingly, the carbon nanotube forest showed microscale patterns defined by the structure of underlying carbon papers. The nanotubes were attached well to the carbon papers and maintained their adhesion under mild ultrasonication in solution. Owing to the direct integration, naturally patterned structure, and good alignment, the carbon nanotubes showed excellent performance as supercapacitors. In aqueous 1 M H2SO4 solution, specific capacitance, energy, and power measured at the current density of 20 A/g were ca. 200 F/g, 20 Wh/kg, and 40 kW/kg, respectively. A specific energy of > 100 Wh/kg was achieved when organic electrolyte was used. Demonstrated facile and direct integration of carbon nanotubes on conductive substrates and their excellent electrochemical properties may hold a great promise for electrochemical energy storage applications. [The Journal of Physical Chemistry C, DOI: 10.1021/jp105498d]

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MAT.O-6**
발표분야: 재료화학분야의 최신 연구동향
발표종류: 구두발표, 발표일시: 금 16:15, 좌장: 방진호

Synthesis and characterization of PEG-modified nanographene oxides (NGOs) and their applications in DNA delivery

Nitin Singhal Kumar, *남좌민

*서울대 화학과 *서울대 화학부*

Graphene is a well-defined two-dimensional structure of carbon atoms. It has received a great deal of attention because of its unique electronic, thermal, and mechanical properties. Potential applications of graphene for nanoelectronics, sensors, and nanocomposites have been actively pursued. The biological applications of graphene and graphene oxide remain relatively unexplored with wide possibilities, however. There are many biological applications possible for a new synthesized material.Here, we report the synthesis of nanographenes from commercially available graphite powder in PEG-conjugated forms for biological applications. DNA is loaded onto the nanographene oxide sheets at a high yield via simple molecular (electrostatic and other specific interaction). Interestingly, the nanographene oxide sheets showed photoluminescence from visible to NIR range, which can be used in cellular imaging with less cytotoxicity compared to carbon nanotube. Cell assay has been performed to find out the fate of DNA in the cells.

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장소: 대구엑스코
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발표분야: 재료화학분야의 최신 연구동향
발표종류: 구두발표, 발표일시: 금 16:40, 좌장: 방진호

NiO-based electrochromic thin films in KOH electrolyte

박대훈

DANSUK industrial Co., LTD.

Since their discovery by Deb at the end of the sixties, electrochromic devices (ECDs), whose optical properties can be modified by an applied voltage, have received significant attention. In particular, in the last decades, great advancements have been achieved in the development of real-world applications, such as rear-view mirrors, helmet visors, car-roof window. A rapid commercialization of smart windows still suffers from issues such as limited durability, neutral color, flexibility, switching speed, etc.. In this presentation the performances of neutral color ECDs will be discussed focusing in particular on the improvement of the counter part NiO. For instance, improved durability of NiO think films was achieved by adding another element/oxide such as Li or TiO_2, or by preparing carbon containing film.

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장소: 대구엑스코
발표코드: **ELEC.O-1**
발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 09:30, 좌장: 표명호

Modification of a Glassy Carbon Electrode with Amine-terminated Dendrimers

김주훈

경희대 화학과

Amine-terminated poly(amidoamine) dendrimers were immobilized on glassy carbon electrodes (GCEs) via electrochemical oxidation of the terminal amine groups of dendrimers. The electrochemical immobilization of dendrimers was confirmed by cyclic voltammetry and X-ray photoelectron spectroscopy. The immobilized dendrimer films were robust and behaved as charge-selective electrochemical gates for oppositely charged redox molecules, i.e. $Ru(NH_3)_6^{3+}$ and $Fe(CN)_6^{3-}$. The immobilization approach was applied to assemble Au dendrimer-encapsulated nanoparticles (Au DENs, 1.5± 0.3 nm) on GCEs, and the resulting Au DEN films showed electrocatalytic activity to hydrazine oxidation.

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장소: 대구엑스코
발표코드: **ELEC.O-2**
발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 09:55, 좌장: 표명호

Photovoltaic effects of CdS nanorods sensitized TiO2 based solar cells using different nanostructured carbon as counter electrodes

Paul Gouri Sankar, *김민우, 김정호, 유종성

*고려대 신소재화학과 *고려대 소재화학과*

Now-a-days quantum dots and nanostructured semiconductors like PbS, InP, CdSe and CdS sensitized solar cells have great research interest due to high conversion efficiency and low production cost.In the present work we have prepared CdS nanorods synthesized TiO2 solar cells and obtained their physical parameters like fill factor (FF), open circuit voltage (Voc), short circuit current (Isc) and conversion efficiency (′). CdS nanorods are synthesized by solvothermal process. Typical diameters of the nanords are varying from 40-50 nm whereas typical lengths are varying from 450-700 nm. These nanorods are uniform throughout their length. Photosensitivities of these CdS nanorods are very high (~106). These CdS nanorods are used to sensitize the TiO2 based solar cells. Here we have used different kind of nanostructured carbon materials (like HCMSC, CMK-3 etc.) as a counter electrode to replace the Pt, which is very expensive. Figure 1 and 2 shows the TEM images and schematic of the CdS sensitized TiO2 solar cells respectively. Various important results will be presented during presentation.

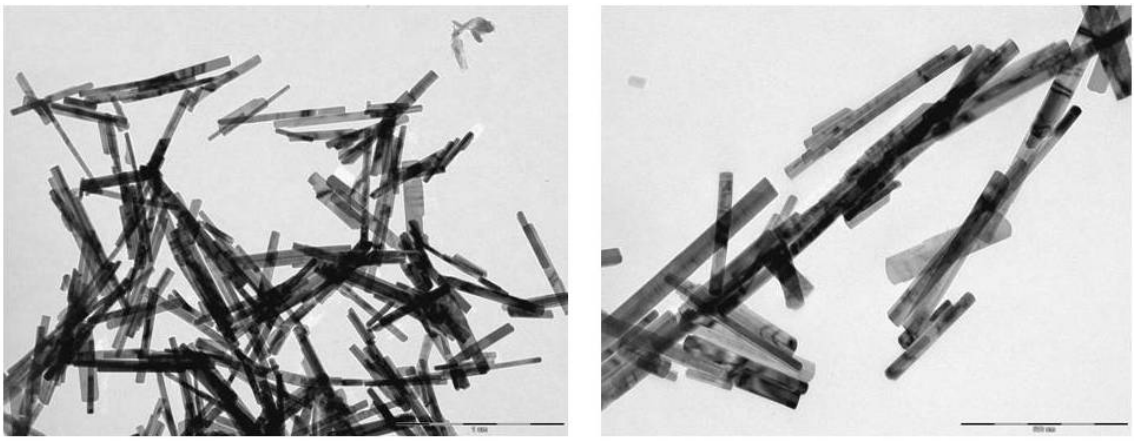

Figure 1: TEM images of CdS nanorods

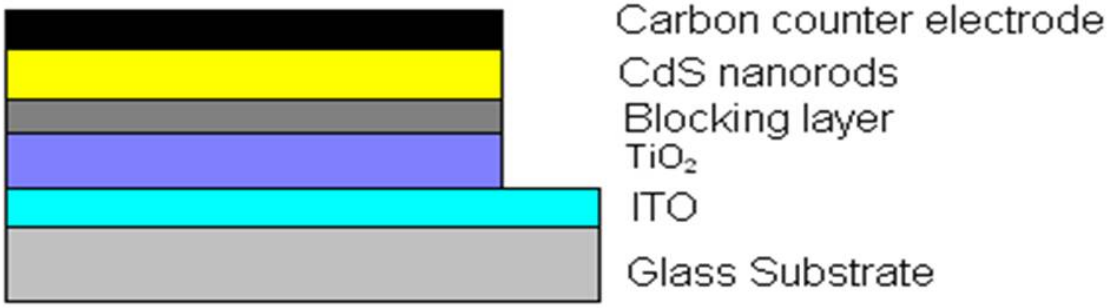

Figure 2: Schematic of CdS nanorods synthesized TiO_2 solar cells

THE KOREAN CHEMICAL SOCIETY

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장소: 대구엑스코
발표코드: **ELEC.O-3**
발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 표명호

Electric Field Enhancements of Solar Cell by Single-Walled Carbon Nanotubes

이원주

KIST(KIST) 태양전지센터

Carbon nanotubes (CNTs) have very attractive properties for solar cells. Their suitable electronic levels, high electric conductivity, and unusual aspect ratio produce the two beneficial effects: (i) the formation of efficient electronic energy structures and (ii) the reduction of interfacial resistance. However, they may not be sufficient to fully explain the significant improvement that is observed. In particular, CNTs are well-known as materials to enhance the electrical field. Therefore, we explore the effect of the CNT layers by measuring the reverse-FE currents and the significant increase in the β value (i.e. the field enhancement factor) that are observed. In addition to these two effects, the enhancement of the electrical field by the CNT layers in solar cells should be considered as another potentially important factor contributing to the improvement of their efficiency. To demonstrate the hypothesis, the superstrate-type Cu(In,Ga)Se2 (CIGS) solar cell, quantum dot-sensitized solar cell (QSSCs), and dye-sensitized solar cells (DSSCs).

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장소: 대구엑스코
발표코드: **ELEC.O-4**
발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이철우

PHOSPHORIC ACID-DOPED PROTON EXCHANGE MEMBRANE OPERATING UNDER ANHYDROUS CONDITION FOR HIGH TEMPERATURE PEMFC

이종원, 김건

고려대 화학과

A proton exchange membrane fuel cell (PEMFC) has been considered as one of the most promising clean energy production systems and as a suitable primary power source for transportation and stationary applications. The commercial application of PEMFC, however, has been limited by some issues such as cost, performance, and stability. Currently, the typical PEMFC uses perfluorosulfonic acid (PFSA) polymer membranes, for instance Nafion and its derivatives. Even though PFSA polymer membranes have demonstrated good performance and stability below 90 °C, it still has several obstacles under elevated temperature conditions. PEMFCs operated under high temperature and anhydrous conditions provide valuable advantages including high tolerance to impurities in the fuels, reduction of the amount of noble metal catalyst on the electrode due to fast reaction kinetics, and construction of compact system without external humidifiers. In the present study, we prepared SDF-F/poly[(N-vinylimidazole)-co-(3-methacryloxypropyl-trimethoxysilane)](poly(VI-co-MPS))/PTFE membrane which is doped with phosphoric acid to form silicate phosphor as a proton carrier. We used porous poly(tetrafluoroethylene) (PTFE) as a reinforcement material. The prepared membrane was characterized by various analytical tools. The thermal stability and conductivity of the membrane were comparable to those of PBI. Single cell test for SDF-F/poly(VI-co-MPS)/PTFE membrane was carried out at 150, 170, and 190 °C to examine the cell performance by measuring cell voltage degradation and phosphoric acid loss..

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장소: 대구엑스코
발표코드: **ELEC.O-5**
발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 11:25, 좌장: 이철우

Increased Pt Stability and Activity for Oxygen Reduction via Alloy of Early Transition Metals

유성종, *성영은

*KIST 연료전지센터 *서울대 화학생물공학부*

Notwithstanding a polymer electrolyte membrane fuel cell (PEMFC) is a promising alternative device to reduce our reliance on environmentally unfriendly fossil fuel, there are several problems that should be overcome to make PEMFC more economically attractive. One of the most pivotal issues of problems is considerable overpotential associated with the slow reaction rate of the oxygen reduction reaction (ORR; ($1/2O_2 + 2(H^+ + e^-) \rightarrow H_2O$)) at the cathode. Other tremendous challenge is the stability for electrochemical reaction, including metal dissolution and surface oxide formation, which occurs intensely in acid medium (< pH 1) at high potential (> 0.8 V). In spite of the significant technological interest in finding active and stable catalyst for ORR condition, the direct experimental inspection of the contributions of the stability involving activity has rarely been investigated in electrochemical reduction of oxygen. Herein we report more active and stable electrocatalytic cathode materials consisting of Pt-based alloys involving late and early transition metals. In particular, we focused on the electronic and lattice-strain effect of the Pt-Y alloys for the purpose of analyzing the activity. To clarify these effects, we introduced a correlation between the d-band structure of Pt induced by its lattice-strain and the ORR activity. In addition, we investigated the stability on Pt-based binary alloy electrodes by applying the calculated *heat of alloy formation* closely relative to the degree of segregation, a descriptor for the stability of electrocatalysts. Our results show keys toward resolving serious problems to make PEMFC economically viable.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **COM-1**
발표분야: 기업과 제품설명회
발표종류: 설명회, 발표일시: 목 14:00, 좌장: 이규양

Future of Chem & Bio Informatics - Past, Current and Future from Desktop Electronic Environment to Enterprise Application

한종수

CambridgeSoft – BITEK CHEMS

The speed of studies have been increased constantly last decades and so does available data/information around researchers. It is critical to utilize the data/information effectively to keep up with the ever increasing research speed and amount of data. Direction of Chem & Bio Informatics will be discussed after current situations are examined.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **COM-2**
발표분야: 기업과 제품설명회
발표종류: 설명회, 발표일시: 목 15:00, 좌장: 이규양

알루미늄 양극산화 나노틀을 이용한 다양한 연구 활동

문학범

(주)넥스트론

주식회사 넥스트론의 제품은 크게 연구용 장치 와 나노틀(Nanotemplate)입니다.학문을 연구하는 연구원 중심의 맞춤형 실험용 반도체 공정장비인 Rapid Thermal Processing System 과 1 micron 최소선폭을 간단한 조작에 의해 쉽게 구현 할 수 있는 Lithographt System 을 개발하여 대학교 연구소 등에 판매하고 있습니다. 규모 있는 기업의 경우 기존 해외의 대형, 고가의 이러한 장치를 많이 사용하고 있지만, 대학의 연구소의 경우 경제적 공간적 제약으로 인해 연구를 위해 이러한 장치에 대한 접근성 어려운 실정입니다. 그래서 넥스트론에서 소형/정밀하면서 사용하기 편리하고, 경제적이면서 필수적인 기능에 충실한 Rapid Thermal Processing System 과 Lithographt System 을 개발하여 연구의 편의를 도모하고자 소개드립니다.제품설명회의 주 내용은 알루미늄 양극산화 나노틀(nanotemplate)을 이용한 다양한 연구 활동입니다. 나노틀의 경우, 고순도의 알루미늄 기판을 양극산화(anodizing) 방법을 이용하여 주기적인 알루미나 나노기공을 형성한 것으로 이러한 나노구조는 단거리 규칙성이 좋을 뿐 아니라 나노기공의 편차도 매우 낮아 나노와이어, 나노마스크, superhydrophobic, 나노필터, display, 광소자 분야등 다양한 연구분야에서 큰 잠재성을 지니고 있는 소재입니다. 넥스트론에서 제조 판매되는 나노틀은 주문자 생산방식으로, 기판의 크기, 나노기공의 크기, 나노기공의 깊이에 따라 다양한 제품을 판매하고 있습니다. 제품설명회 홍보 내용은 AAO(anodic aluminium oxide)를 연구하는 대학원생들을 대상으로 AAO 개발 초기 넥스트론에서 경험한 사례 중심으로 알루미늄 기판준비, AAO 세부공정, 최근 AAO 응용연구분야 등으로 할 계획입니다.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **COM-3**

발표분야: 기업과 제품설명회

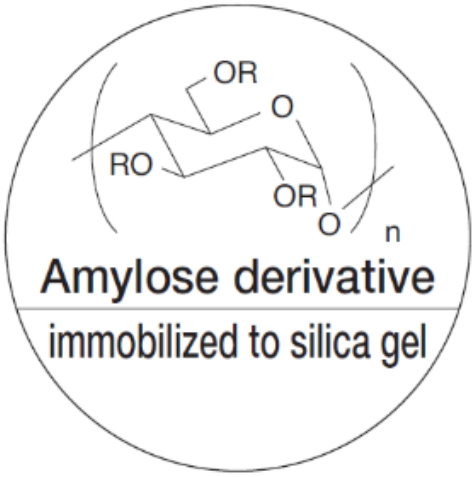
발표종류: 설명회, 발표일시: 목 15:40, 좌장: 이규양

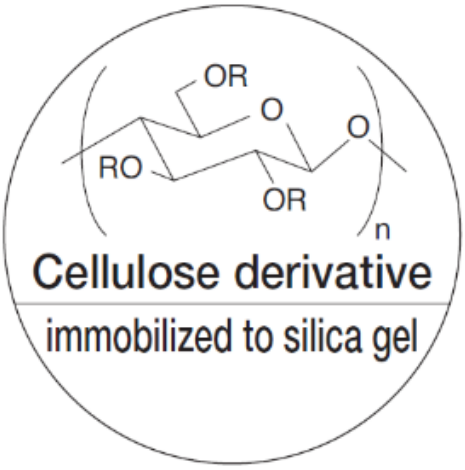
라세믹 화합물 분리시 탁월한 분리능과 폭 넓은 응용범위를 제공하는 Daicel사 신제품 소개

안성용

(주)알에스텍

거울상 이성질체 화합물의 가장 효과적인 분리는 다당류(셀루로스와 아밀로오스)에서 유도된 카이랄 칼럼을 사용했을 때 확인하실 수 있습니다. 다당류 유도체 CSPs 개발을 통해 다양한 칼럼이 있기에 폭 넓은 응용 범위를 제공합니다. Daicel 사의 칼럼은 현재 많은 기업, 연구소 및 대학에서 사용 중입니다. 이러한 연구원분들의 기대에 부응하고자 신규 제품을 출시하였습니다. 빠른 분석 시간, 높은 분리능, 높은 효율을 가지는 칼럼을 제공해 드리고자 최근엔 입자 크기 3μm 인 칼럼을 개발 하였습니다. 공유결합형, 코팅 타입 CSPs 그리고 protein type CSPs 의 장점과 응용 범위에 대해서 설명드릴 예정입니다.





일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **COM-4**
발표분야: 기업과 제품설명회
발표종류: 설명회, 발표일시: 목 16:10, 좌장: 이규양

(주) 피어슨에듀케이션코리아 소개 및 제품 설명

최성원

(주)피어슨에듀케이션코리아

피어슨 코리아는 세계적인 교육출판 그룹인 피어슨에듀케이션의 한국지사입니다. Ⅰ. 회사소개 전세계적으로 1 억명의 교육을 도와주는 피어슨은 교육 출판업계의 세계적 리더입니다.자신들만의 방법으로 진도를 나아가며 학습하는 학생들을 도와줄 수 있는 과학적 연구를 기반으로한 서적과 디지털 프로그램들을 제공합니다.Ⅱ. 제품소개 화학분야 교재 및 온라인 교육 솔루션 및 이러닝 솔루션 (MasteringChemistry, ACE Organic, ChemistryPlace 등) 소개

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **COM-5**

발표분야: 기업과 제품설명회

발표종류: 설명회, 발표일시: 목 16:30, 좌장: 이규양

FT-NMR 악세사리, FT-IR ATR 제품 홍보

하태현

비케이인스트루먼트

FT-NMR 악세사리, FT-IR ATR 과 그와 관련한 제품 홍보

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **COM-6**

발표분야: 기업과 제품설명회

발표종류: 설명회, 발표일시: 목 16:50, 좌장: 이규양

EYELA 신형 Rotary Evaporator System, Organic Synthesize System 소개

최준호

(주)선일아이라

실험실 환경과 실험자의 건강을 고려해 개발한 신형 Rotary Evaporator System 소개와 Organic Synthesize System(Microwave, Parallel) 특징 및 사용법 소개

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **COM-7**
발표분야: 기업과 제품설명회
발표종류: 설명회, 발표일시: 목 17:10, 좌장: 이규양

Pipeline Pilot™ Enabling Collaboration in Research & Development Organizations

김성곤

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Vinyl-addition Polymerization of Norbornene Monomer Bearing 4,4'-bis(9-carbazolyl)-biphenyl Side Groups : A New Class of Host Material for Highly Efficient Green PhOLEDs

박준하, *이민형, 도영규

*KAIST 화학과 *울산대 화학과*

The soluble polynorbornene bearing pendant 4,4'-bis(9-carbazolyl)-biphenyl (CBP) side groups was prepared by the vinyl addition polymerization of norbornene monomer with Pd(II) catalyst in combination with 1-octene chain transfer agent (CTA). The polynorbornene exhibits very high glass transition temperature (T_g > 360 ^oC) and good film forming ability. When being incorporated into emissive layer as the host doped with *fac*-$Ir(ppy)_3$ through solution process, the polymer displayed excellent host ability comparable to that of the molecular CBP processed by vacuum deposition method. Details of synthesis, characterization, and host properties of the polymer will be discussed.

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zinc glutarate and its derivatives in chemical fixation of CO2 into polycarbonates

최준만, *이문호, *박삼대, *김진철, *김동민, *정정운, *안병철, *권원상, *김경태, *김미희, *고용기

*포항공과대 화학관 *포항공과대 화학과*

A heterogeneous zinc glutarate (ZnGA) catalyst and its derivatives were prepared from various zinc and glutarate sources. The ZnGA single crystals (sc-ZnGA), with a monoclinic lattice unit cell, as determined by X-ray single-crystal structural analysis. The structural details of the ZnGA catalyst are crucial in helping to elucidate its activity in the copolymerization reactions between carbon dioxide (CO2) and alkylene oxides. The activity of the ZnGA catalyst in the copolymerization of CO2 and PO was found to depend on the zinc source used, and its ability to produce a catalyst of large surface area and high crystallinity (≥77%). Modification of the glutarate ligand with electron-donating or withdrawing substituents failed to enhance the ZnGA catalyst activity further, indicating that glutarate is the best ligand for the Zn metal ion to achieve a high catalytic activity in the CO2 copolymerization with PO.

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Unipolar and Bipolar Bistable Characteristics of Polyimide with Diphenylaminobenzylidenylimine Moieties

권원상, 김경태, 박삼대, 김동민, 김진철, 고용기, 정정운, 노예철, 안병철, 김미희, 정성민, *최준만, 이문호

*포항공과대 화학과 *포항공과대 화학관*

This study reports the synthesis and properties (in particular, the electrical switching characteristics) of a new high-performance polyimide (PI),poly(3,3´-di(4-(diphenylamino)benzylidenyliminoethoxy)-4,4´-biphenylenehexafluoroisopropylidenediphthalimide) (6F-HAB-TPAIE PI). This PI polymer bears diphenylaminobenzylidenylimine moieties as side groups and is dimensionally stable up to 280 °C and thermally stable up to 440 °C. In devices fabricated with the PI polymer as an active memory layer, the active PI polymer was found to operate at less than ±2 V in electrically bistable unipolar and bipolar switching modes by controlling the compliance current. The PI polymer layer exhibits repeatable writing-reading-erasing capability with high reliability in ambient air conditions as well as at high temperatures up to 130 °C. This PI polymer also exhibits a high ON/OFF current ratio up to 109. The observed nonvolatile memory behaviors are due to Schottky emission and local filament formation.

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Synthesis and purification of PAMAM(generation 0)-dexamethasone conjugate for gene delivery in vitro

김태훈, 최혜, 최윤희, 안난영, 최준식

충남대 생화학과

Efficient targeting of DNA to the nucleus is a prerequisite for effective gene therapy. Dexamethasone, a glucocorticoid steroid, can dilate the nuclear pore complexes and translocate into the nucleus when it bound to its glucocorticoid receptor. It is suggested that the transport of DNA to nucleus may be facilitated by glucocorticoid. In this study, dexamethasone was conjugated to PAMAM dendrimer (generation 0) for efficient translocation of the polymer/DNA complex into the nucleus and the effect of the conjugation was investigated. PAMAM-dexamethasone conjugate was synthesized by one-step reaction using the Traut's reagent. To make a liposomal solution for gene delivery, DOPE was used as a fusogenic helper lipid. In gel retardation assay, the PAMAM-dexamethasone conjugate/DOPE liposome/DNA complex was completely retarded at 8:1 N/P (nitrogen/phosphate) ratio. The average size distribution and ζ-potential value of the complex were measured at 8:1N/P ratio. In vitro transfection assay showed that the PAMAM-dexamethasone conjugate/DOPE liposome/DNA complex had higher gene delivery efficiency compared to PAMAM/DNA complex. And PAMAM-dexamethasone conjugate/DOPE liposome showed lowest toxicity compared to PAMAM, PEI 25kD and Lipofectamine 2000®. These results indicated that with efficient nuclear translocation and low cytotoxicity, PAMAM (generation 0)-dexamethasone conjugate/DOPE liposome has a potential to be used as an efficient gene carrier for gene therapy.

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Photoinitiated RAFT polymerization in fluoroalcohol; Simultaneous control of molecular weight and stereochemistry

함민경

숭실대 유기신소재파이버공학과

Since the active radicals has low energy barrier between two enantiomers, it is very difficult to control stereochemistry in radical polymerization. Protic solvents such as fluoroalcohols are known to be efficient for controlling stereochemistry in radical polymerization of vinylesters. Another approach to improve stereoregularity of the prepared polymer is lowering polymerization temperature. Although radical addition and fragmentation chain transfer (RAFT) process is effective to prepare polymers with specific molecular weight, it usually uses thermal initiators as a radical source, which make it difficult to lower the polymerization temperature. In this work, we used photoinitiation process to generate radicals. RAFT process of vinyl acetate in fluoroalcohol using photoinitiation process was conducted and the effect of fluoroalcohol and reaction temperature on the stereospecificity of the prepared polymer was studied.

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Novel polypeptide-based polymeric micelles of poly(ethylene glycol)-poly(S-dodecyl-L-cysteine) for solubilization of hydrophobic drug molecules

김현철, 정상원, 김은주

대구경북과학기술원 나노바이오연구부

Novel amphiphilic diblock copolymers composed of poly(ethylene glycol) and poly(S-dodecyl-L-cysteine) were synthesized and the resulting polymeric micelles as drug carries were investigated. Methoxy-poly(ethylene glycol)-b-poly(S-dodecyl-L-cysteine) (mPEG-b-PDC) was prepared by ring opening polymerization of S-dodecyl-L-cysteine N-carboxyanhydride using methoxy-poly(ethylene glycol)-amine and the structure was characterized by means of 1H-NMR, FT-IR, and GPC measurements. The prepared copolymers formed polymeric micelles in water as evidenced by the solubilization of pyrene and dynamic light scattering measurements. The critical micelle concentration (CMC) of the amphiphilic copolymers was in the range of less than 10 mg/L. The drug loading content and entrapment efficiency of the polymeric micelles were estimated using indomethacin as a model drug with various ratios of drug and polymer. mPEG-b-PDC micelles exhibited a bimodal distribution with peaks at around 20±10 and 100±30 nm. The polymeric micelles showed the tendency to aggregate with a longer hydrophobic PDC block or a loading of hydrophobic IMC into the micelles. The toxicity of mPEG-b-PDC polymeric micelles was performed using L929 mouse fibroblast cells and the low toxicity supports their potential biomedical use as drug delivery vehicles.

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Molecular design for optimized FRET to dye-labeled DNA in polymer-based DNA detection

김보람, *심홍구, **우한영

*부산대 나노융합기술학과 *KAIST 화학과 **부산대 나노기술대학 나노정보소재공학과*

Cationic conjugated polymers (CCPs) with different charge density per repeat unit were synthesized and studied as a fluorescence resonance energy transfer (FRET) donor to fluorescein–labeled single stranded DNA (ssDNA-Fl). The CCPs show similar absorption and emission spectra in water but obviously different solubility and the resulting optical properties such as PL quantum yield in aqueous solution. The FRET-induced Fl signal amplification was investigated in detail in terms of charge density of the polymers, water-solubility and the resulting spectroscopic properties, the electrostatic complexation and the photo-induced charge transfer (PCT) quenching in the polymer/ssDNA-Fl complex.

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Preparation of double wall microcapsules containing octadecane to improve of thermal stability

김성훈, *조창기

*한양대 섬유고분자공학과 *한양대 응용화공생명공학부*

Melamine-formaldehyde (M-F) microcapsules containing octadecane as a phase change material (PCM) were modified with diisocyanate to improve their thermal stability. Modification by post reaction at the outside of the capsules wall was made by addition of diisocyanate dispersion after the completion of encapsulation reaction. First, encapsulation by in situ polymerization using melamine-formaldehyde as shell materials was controlled by pH through phosphate-citric acid buffer solution. Second, dispersion of diisocyanate was added into M-F microcapsules emulsion. In this study, thermal stability and encapsulation efficiency were analyzed through TGA, DSC. SEM was used to characterize the morphology of microcapsules.

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Characterization of heat treated Nafion® membranes for PEMFC performance

김정민, *조창기

*한양대 섬유고분자공학과 *한양대 응용화공생명공학부*

Nafion membrane has many desirable properties as a proton-conducting electrolyte, such as high mechanical strength and dimensional stability, good chemical stability as well as high proton conductivity under high-humidity conditions. However, the membrane has poor ionic conductivity at low humidity and/or elevated temperatures, which limits the possibility of operating fuel cells at these conditions.The purpose of this study is to obtain detailed information of the Nafion membranes decreasing ionic conductivity at high temperature. The differences between before and after high temperature aging were investigated by the proton conductivity, ion exchange capacity (IEC), water uptake, and thermal stability. Detailed results will be presented.

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Preparation of crosslinkable N-sulfonated poly(m-phenylene isophthalamide)(Nomex) and their Characterization for PEMFC Membrane

김선미, *조창기

*한양대 분자시스템공학과 *한양대 응용화공생명공학부*

Poly(m-phenylene isophthalamide) (Nomex) shows high temperature stability and strength, making it attractive in many applications. However, its processability is quite limited due to hydrogen bonding, poor solubility in common organic solvents, and high melting point. In this study, N-substituted Nomex was synthesized to improve its processabilities and to check the possibility as a membrane material for fuel cell application. The synthesized polymers were transformed into crosslinked proton exchange membranes. The prepared membranes were characterized in terms of the proton conductivity, ion exchange capacity(IEC), water uptake, methanol permeability, and thermal stability. Detailed results will be presented.

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Properties of multivalent metal ions-induced hydrogels

박수정, *김민관, 정상원

*대구경북과학기술원 나노바이오연구부 *대구경북과학기술원 나노바이오연구부, 경북대*

The properties of reverse thermal hydrogels formed from mixing poly (propylene oxide)-b-poly(ethylene oxide)-b-poly(propylene oxide)-bisphosphate (PO_4^{2-}-PPO-PEO-PPO-PO_4^{2-}) are described. The reverse Pluronic triblock copolymer-bisphosphate, which did not form a hydrogel in water, underwent sol-to-gel transition immediately upon addition of multivalent metal ions such as Ca^{2+}, Cu^{2+}, Zn^{2+}, Mg^{2+}, Fe^{2+}, and Fe^{3+}. The phase transition and the mechanical properties of the hydrogels were investigated depending on metal ions, additives, concentration, and copolymer composition. The gel stability and in vitro drug release were studied by variation of pH and salt concentration. The gel formation mechanism is to be discussed.Keywords: Hydrogel, Reverse Pluronic, Sol-to-gel transition

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Reactivity of the meta-activated nucleophilic aromatic substitution reaction

김선달, *정임식, 김상율

*KAIST 화학과 *KRIBB 바이오나노연구센터*

Nucleophilic aromatic substitution (S_NAr) reaction is very effective for the formation of aromatic ether linkages, which are found in many natural and synthetic products. The S_NAr reaction requires the leaving group activated with an electron withdrawing group at the ortho and/or para position, which stabilize the negative charge developed during the transition state through conjugation. We have reported that the trifluoromethyl activating group located at meta position to the nitro leaving group is active enough to obtain high-molecular weight poly(arylene ether)s. In this study, the reaction behaviors of the meta-activated S_NAr reaction using two trifluoromethyl activating groups have been investigated, and the detailed reactivity study results will be presented.

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Effect of Unsymmetrical Spiro Structure on the Partially Aliphatic Polyimides

유환철, *Vijay Kumar S, **Jiyoung Choi, **Kazuaki Kudo, 정찬문

*연세대 화학과 *Department of Chemistry, Yonsei University **Institute of Industrial Science, The University of Tokyo*

The effect of monomer structure on polymer properties was studied for partially aliphatic polyimides based on alicyclic dianhydrides and aromatic diamines. Structures of the polyimides were confirmed by H1-NMR and FT-IR spectra. Solubility of the polyimides was tested in various organic solvents and thermal property of the polyimides was investigated by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The results were correlated with the molecular arrangement of the polyimides that was studied by wide-angle X-ray diffraction (WAXD). All these properties are understood on the basis of the structure of the polymimides. UV-visible spectra were obtained to evaluate the transparency of the polyimides.

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Analysis of PS-*g*-PI graft copolymer using LCCC x LCCC

이효준, 안선영, 장태현

포항공과대 화학과

Graft copolymer is a polymer having side chains composed of different monomers to that of the main chain. Since the backbone and graft chains are generally incompatible, most graft copolymers are multiphase materials exhibiting unique and interesting morphologies. Usually graft copolymers are characterized by size exclusion chromatography (SEC). But it is not enough to characterize graft copolymers precisely since they often include various side products. In this study, we analyzed PS-*g*-PI graft copolymers with 2D-LC by combining two liquid chromatography at the critical condition (LCCC). The polystyrene-*graft*-polyisoprene (PS-*g*-PI) was prepared by tailored anionic polymerization to yield precisely spaced graft chains. In so doing, imperfect stoichiometry and side reactions leads to inhomogeneity in backbone length as well as in the number of grafts. LCCC permits the characterization of individual blocks of copolymer by making one block chromatographically "invisible". The first-dimension separates PS-*g*-PI according to the PI block length while the second-dimension separates PS-*g*-PI according to the PS block length, each of which is at the critical condition of PS and PI, respectively.

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Effect of addition of crystalline material to the critical transformation temperature of polymeric PTC

이상범, *오응주

*명지대 전도성 고분자 연구실 *명지대 화학과*

Up to now, polyurethane / carbon black / stearic acid showed the lowest critical transformation temperature (Tc) of 70℃ among polymeric PTC composites. This is due to the expansion in volume of stearic acid. In this study, palmitic acid and myristic acid which shows lower Tc than stearic acid were used to make the composite and the effect of those on the Tc. Programmable oven and digital multimeter were used to measure the temperature dependence of resistivity.Melting point of palmitic acid, myristic acid and Tc of the composite were measured by DSC. From the SEM images of composites, the degree of dispersion will be discussed.

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Synthesis of graphene-polypyrrole composite and its properties

김진화, 박희수, 오응주

명지대 화학과

Many researches have been carried out to improve the processibility of graphene for last few years. One method to prevent graphene from agglomerating is coating of graphene with conducting polymer. In this study, graphene dispersion was prepared in aqueous medium in which surfactant, DBSA was added as a dopant. Then pyrrole was polymerized in the dispersion. XRD was used to confirm the formation of graphene. FT-IR, TGA, SEM, conductivity were measured with graphene-polypyrrole composite powder. From the results, chemical and physical properties of graphene nanosheets-polypyrrole composite will be discussed.

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Poly(3,4-ehtylenedioxythiophene) nanotube syhthesized by peptide nanowire

김방한, 이미희, 오웅주

명지대 화학과

Several methods have been used to synthesize the conducting polymer nanostructure such as reverse microemulsion, solid / liquid template synthesis etc. In this study, PEDOT nanostructure was prepared using self assembled peptide as a template and its structure was investigated. Self assembled peptide nanorod structure was formed by exposure of glass substrate coated with diphenylalanine to water vapor. Then PEDOT was synthsized on nanostructure by vapor deposition of EDOT. PEDOT nanotube was prepared by removal of template. Effect of the type of oxidants and preparation procedure on the structure of PEDOT nanotube was investigated. And chemical and physical properties will be discussed.

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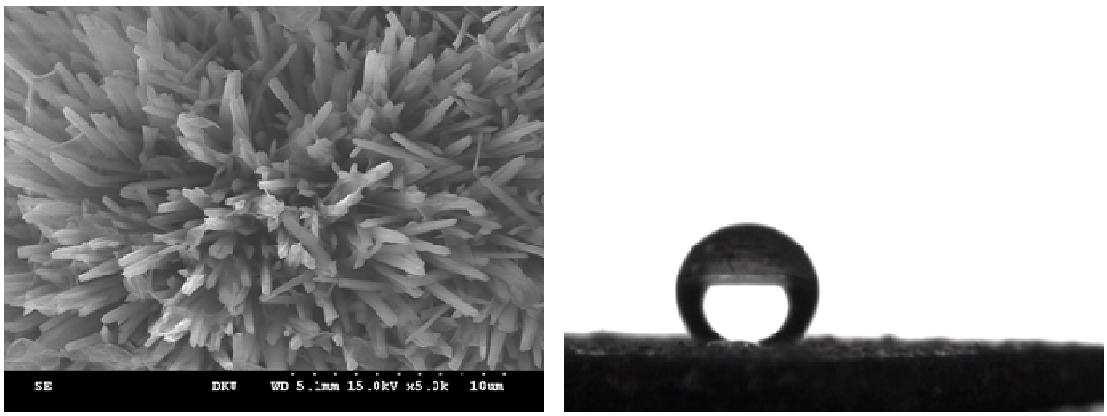
Preparation of Super-Hydrophobic Surface Based on Nanorod Structure on Magnesium Surface

박연화, 안용현

단국대 화학과

The wettability of solid surfaces is of great interest in daily life and industry. Wettability is controlled by both the geometrical structure of a surface and a low surface energy material coating. A superhydrophobic surface is satisfied with a water contact angle of more than 150° and a sliding angle of less than 10°. In nature, this is the lotus effect. We synthesized alkyl-and aryl urea silane and diphosphono alkane derivatives. The urea silane derivatives were polymerized in the presence of 1,6-diphosphono alkane to form the nanorod structure. The reaction mixture was used to fabricate the superhydrophobic surface of magnesium. The magnesium flakes were dipped into the reaction mixture. Depend on dipping times the length of nanorod was changed. The hydrophobic surfaced that obtained by coated with nanoroad structure were analyzed with FE-SEM, XPS and optical contact angle meter.



FE-SEM image of the coating surface and the profile of a water droplet on the suface.

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1-Amino-4-methyl piperazine을 이용한 은 나노 콜로이드 용액의 제조

박헌수, 공명선

단국대 나노바이오의과학과

첨단 소재인 나노복합재료는 단일 소재로서는 달성되어질 수 없는 단점을 극복하기 위해 또 다른 하나의 나노소재 분야 및 나노기술로서 그 중요성이 대두되고 있는 가운데 많은 연구가 이루어지고 있다. 은 콜로이드 용액은 전극재료, 부식 방지막 및 센서 개발 등 산업적인 측면 및 나노 화학 연구에 많은 도움을 줄 것으로 기대되어진다. 최근 많은 영역에서 은 나노 입자를 제조할 때 안정화의 필요성을 강조되는데, 본 실험은 nano size 의 은 콜로이드 용액을 얻기 위하여 1-amino-4-methylpiperazine 를 환원제 및 안정제로 사용하였다. 1-amino- 4-methyl piperazine 은 따로 안정제를 쓰지 않아도 콜로이드된 Ag composite 의 size 를 일정하게 조절하기가 용이하다. 본 연구는 Ag-Cabarmate Complex 의 농도 및 시간 온도와 같은 다양한 인자들을 달리하여 Ag particle 의 입자형상 및 Size 를 제어하기 위한 것으로, 이를 통해 얻어진 입자들은 TEM, XRD, UV-vis, fad-Mass 등의 분석법들을 통해 분석하였다.

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Characterization of Multi-arms Star Polystyrenes by Small Angle X-ray Scattering using Synchrotron Radiation Source

정성민, 노예철, 안병철, 박삼대, 김진철, 김동민, 정정운, 권원상, 김경태, 김미희, 고용기, *최준만, 이문호, **Tomoya Higashihara, **Akira Hirao

*포항공과대 화학과 *포항공과대 화학관 **Tokyo Institute of Technology*

We have synthesized well-defined multiarmed star polystyrenes, with 6, 9, 17, 33, and 57 arms, and studied their molecular shapes and structural characteristics in a good solvent (tetrahydrofuran at 25 °C) and in a theta (Θ) solvent (cyclohexane at 35 °C) by small-angle X-ray scattering (SAXS) using a synchrotron radiation source. Analysis of the SAXS data provided a detailed characterization of the molecular shapes, including the contributions of the blob morphology of the arms, the radius of gyration, the paired distance distribution, the radial electron density distribution, and the Zimm–Stockmayer and Roovers g-factor, for the multiarmed star polystyrenes. In particular, the molecular shapes of the star polystyrenes were found to change from a fuzzy ellipsoid, for the 6-armed polystyrene, to a fuzzy sphere, for the 57-armed polystyrene, with an increasing number of arms. The ellipsoidal character of the star polystyrenes with fewer arms may originate from the extended anisotropically branched architecture at the center of the molecule. The arms of the star polystyrenes were found to be more extended than those of the linear polystyrenes. Furthermore, the degree of chain extension in the arms increased with the number of arms.

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MRI nanoprobes encapsulated by poly-D,L-gamma glutamic acid(γ-PGA) based polymeric micelle

최두열, *성문희

*국민대 생명나노화학과 *국민대 화학과*

In this research, we have synthesized biocompatible polymer micelles encapsulating superparamagnetic manganese-iron oxide nanoparticles (Mn-SPIONs). γ-PGA based amphiphilic polymers, cetyl(hexadecyl)-poly(D,L-gamma glutamic acid)-poly(ethylene glycol), were synthesized through sequential alkyl halide esterification and EDC-NHS coupling for NH-PEG conjugation with γ-PGA . Hydrophobically synthesized Mn-SPIONs were encapsulated by the amphiphilic polymers through self-assembly and successfully dispersed in aqueous phase. These magnetic nanoparticles were finally applied for the labeling of immune cells. Taken together, the Mn-SPIONs encapsulated by biocompatible polymer micelles can be used as highly efficient T2-weighted magnetic resonance imaging contrast probes for immune cell tracing.

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Study of micelle-like arrangement of selenious acid doped polyaniline

송예리, 손대원

한양대 화학과

Conventional polyaniline (PANI) has been shown to have a lot of promising potential applications due to its tunable conductivity, good environmental stability and potential for applications in electronic devices and chemical sensors. Unlike other conjugated polymers, PANI has a simple and reversible acid/base doping/dedoping chemistry, enabling control over properties such as free volume, solubility, electrical conductivity, and optical activity. In our laboratory we have observed morphology transition of selenious acid doped polyaniline and its properties. For the study of micelle-like arrangements of selenious aicd – aniline salt through an acid/base reaction, dynamic light scattering (DLS) experiments were performed by varying dopant – monomer mole ratio. AFM and UV-vis were also used for characterization.

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A study of the behavior of star-shaped poly(ethylene oxide) at the air/water interface

전민희, 손대원

한양대 화학과

Poly(ethylene oxide) (PEO) is particularly attractive in the field of pharmaceutical and biomedical applications. Biologically active molecules can be immobilized on the end of the PEO arms.An objective of this study is to identify the properties and two dimensional behavior of 4-arm amine terminated PEOs which are used in the component of three dimensional biocompatible tetra-PEG gel. To reveal our curiosity, we used the Langmuir-Blodgett (LB) technique which allows for the fabrication of ordered monolayers and organized molecular assemblies with well-defined molecular orientation on a desired substrate. To understand the behavior of a star polymer, 4-arm amine terminated poly(ethylene oxide), at the air/water interface, we measured the surface pressure measurements, the surface pressure-area (Π−A) isotherm and compression-expansion hysteresis measurement. As a result, although PEO is a water soluble polymer, isotherms were stable and reproducible at the air/water interface and showed no hysteresis. We guessed that such a surface-active polymer with high molecular weight poly(ethylene oxide), even though water soluble, can form well-spread films at the air/water interface. Further studies of these molecules by Atomic Force Microscopy (AFM) and Brewster Angle Microscopy (BAM) show the well dispersed monolayer at the air/water interface and on the solid substrate.X-ray reflectometry was used to characterize star-shaped polymers on solid substrate. The data of electron density profile, the thickness of layer, and the interfacial roughness support the uniformity of 4-arm PEO monolayers.

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Preparation, characterization of purified Imogolite and its capacity of gas storage

박혜미, 손대원

한양대 화학과

Imogolite is a hydrous aluminosilicate nanofiber with the general formula of [Al2O3•SiO2•2H2O], which is one of porous materials. The porous properties were studied by BET methods with N2/77K adsorption isotherms. The specific surface area of Imogolite is 213.96m2/g. Because of its specific properties, Imogolite is able to absorb and store gases. To measure the capacity of gas storage clearly, byproducts made on synthesis process of Imogolite should be removed by purification process included centrifugation and dialysis. The purified Imogolite is characterized by powder X-ray diffraction (powder XRD), Fourier transform infrared (FT-IR) spectroscopy and transmission electron microscopy (TEM). Especially XRD data show that the purification process works well to separate the pure Imogolite. The capacity of gas storage for Imogolite is measured by High-Pressure (HP, Bel Japan, INC.).

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Amphiphilic cyclotriphosphazenes grafted with branched oligopeptides

CUI JINXIN, Vithal Jadhav, 전용주, *손연수

*이화여대 화학·나노과학과 *씨앤팜 부설연구소*

Branched oligopeptides prepared by coupling a very hydrophobic aspartic diamino acid ethyl ester such as $Asp(LeuEt)_2$, $Asp(IleEt)_2$ and $Asp(PheEt)_2$ to glycine or glycylphenylalanine were grafted to the cyclotriphosphazene backbone bearing an equimolar hydrophilic poly(ethylene glycol) (PEG). The properties of the resultant amphiphiles were examined in comparison with those of the linear oligopeptide analogues previously reported. All cyclic phosphazene trimers grafted with the branched tetra- and pentapeptides displayed a normal trend of thermosensitivity depending on their hydrophilic to hydrophobic balance, but the stability and particle size of their micelles were found to be greatly dependent on the fine structure of the branched oligopeptides grafted. The trimers bearing branched tetrapeptides with a low hydrophobicity were found to form unstable micelles initially, which reassemble into thermodynamically more stable polymersomes.

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Synthesis and Properties of Thiophene-Pyrrole-Thiophene based Broad Absorption Alternating Copolymers for Solar cells Applications

V. Tamilavan, 현명호

부산대 화학과

Two new alternating copolymers namely poly[4,7-bis(3-octylthiophen-2-yl)benzothiadiazole-co-1-(2,6-diisopropylphenyl)-2,5-di(2-thienyl)pyrrole (PTPTTBT-P1) and poly[4,7-bis(3-octylthiophen-2-yl)benzothiadiazole-co-1-(p-octylphenyl)-2,5-di(2-thienyl)pyrrole (PTPTTBT-P2) were synthesized via Suzuki polymerization reaction. The absorption ranges of the two polymers were quite broad (250–650 nm for PTPTTBT-P1 and 250–1000 nm for PTPTTBT-P2). The optical band gaps of the copolymers were calculated from the onset absorption wavelength of the film state absorption spectrum, which is 1.94 and 1.29 eV, respectively. Under 100 mW/cm2 of AM 1.5 white-light illumination, bulk heterojunction PSC devices containing an active layer of electron donor polymers mixed with electron acceptor [6,6]-phenyl C70-butyric acid methyl ester (PC70BM) in the weight ratio of 1:4 were investigated. The PSC device containing PTPTTBT-P1 gave the best preliminary result with an open-circuit voltage of 0.52 V, a short-circuit current of 4.67 mA/cm2, and a fill factor of 0.30, offering an overall power conversion efficiency (PCE) of 0.74%.

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Tunable Optical Properties in Block Copolymer/Inorganic Nanocomposites

김성남, 허성우, 고재윤, 김승빈

포항공과대 화학과

Block copolymer (BCP) templates have been attention for its potential to self-assembly into highly-ordered nanostructures over large surface area. These nanostructures could be used to produce the meta-material for plasmonic and sensitive photonic devices. Here, we prepared vertically oriented cylindrical microdomains in thick films by PS-b-P4VP micelles and solvent annealing. These templates were immersed to inorganic salt solutions such as $HAuCl_4$, $AgNO_3$ and $PtCl_4$ in Methanol. The nanoparticles (NPs) could be formed by chemical and photochemical reducing. Ag, Au and Pt NPs were selectively located in the P4VP building blocks. The BCP/NPs ratio could be relatively estimated by FTIR spectroscopy. The controlled BCP/NPs ratio and UV-irradiation time induced a broad tunability of surface plasmon band of these NPs.

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MWCNT와 은 나노 입자를 이용한 protein carrier 개발 및 특성 조사

박형석, *신원상, 공명선

*단국대 나노바이오의과학과 *단국대 나노바이오의과학*

첨단 소재로서 나노복합재료는 단일 소재로써는 달성되어질 수 없는 단점을 극복하기 위해 또 다른 하나의 나노소재 분야 및 나노기술로서 그 중요성이 대두되고 있는 가운데 많은 연구가 이루어지고 있다. 은 콜로이드 용액은 전극재료, 부식 방지막 및 센서 개발 등 산업적인 측면 및 나노 화학 연구에 많은 도움을 줄 것으로 기대되어진다. 최근 많은 영역에서 은 나노 입자를 제조할 때 안정화의 필요성을 강조되는데, 본 실험은 nano size 의 은 콜로이드 용액을 얻기 위하여 1-amino-4-methylpiperazine 를 환원제 및 안정제로 사용하였다. 1-amino- 4-methyl piperazine 은 따로 안정제를 쓰지 않아도 콜로이드된 Ag composite 의 size 를 일정하게 조절하기가 용이하다. 본 연구는 Ag-Cabarmate Complex 의 농도 및 시간 온도와 같은 다양한 인자들을 달리하여 Ag particle 의 입자형상 및 Size 를 제어하기 위한 것으로, 이를 통해 얻어진 입자들은 TEM, XRD, UV-vis, fad-Mass 등의 분석법들을 통해 분석하였다.

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Highly Efficient White Organic Light Emitting Diodes from Single Molecule based on Naphthalene Core

김동원, *박영일, **이기호, *박종욱, 이지훈

*충주대 나노고분자공학과 *가톨릭대 화학과 **고등과학원 계산과학부*

Recently, the applications of p-conjugated organic materials in electronic industryare occurring conspicuously as useful in display field using organic light-emitting diodes(OLEDs). In particular, white organic light-emitting diodes (WOLEDs) are enteringspotlight extensively are drawing massive attention since they can be potentially appliedto low cost large area backlight for flat panel displays and solid lighting sources. Toproduce white emission, various methods are under development. For instance, inOLEDs using small molecules, multilayered device structure obtained throughconsecutive evaporation of each layer in red, green and blue respectively is used toproduce white emission. In such methods, charge blockers are required. However, since suchblockers cause high driving voltage and low efficiency, this method cannot be thatdesirable one. To quote another method, in OLEDs using polymer, 2 to 3 fluorescent orphosphorescent materials are used through blending as guest material in blue emissive ornon-active polymer host in general. However, this method involves many seriousproblems like phase separation between host polymer and guest molecules by heat,discoloring by energy transfer toward chromophore with lower energy, or decrease ofdevice efficiency by the difficulty of refining above all. Compared with such multiemitting-component WOLEDs, single-emitting component WOLED could have manystrong points like better efficiency, better stability, better reproducibility and simplerfabrication process. However, developments of materials that produce white emissionwith single molecule alone are very negligible, and furthermore, there are barely anyreports found on materials with device stability and high performance while with purewhite light emission. We report herein the design and syntheses of the new naphthalene-cored emitters,and its white electroluminescent properties

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액츄에이터에서의 전극물질 두께에 따른 특성평가

이현준, 권병국

한국산업기술대 신소재공학과

최근 전기활성고분자 (Electroactive polymer; EAP)는 비교적 신생의 연구 분야로서 전도성 고분자를 이용하여 생체근육과 유사한 큰 변위를 낼 수 있는 재료 고유의 특성으로 인하여 매우 관심이 고조되는 분야이다. 전도성 고분자를 전해질과 반응시키고 전압을 인가하면 전도성 고분자가 산화 상태가 되며 (+)전하를 띄고, 전해질 내의 (-)전하가 용매와 함께 전도성 고분자로 이동하여 전도성 고분자는 팽윤되는 현상에 의해 필름 형태의 전도성 고분자의 부피 팽창과 수축으로 인하여 구동한다. 이 전도성 고분자가 전압의 인가에 따라 산화, 환원이 반복되면 전도성 고분자는 부피 팽창과 수축이 따르고 이것이 EAP 의 구동원리가 된다. 이러한 전도성 고분자를 이용하여 EAP 에 관한 많은 연구가 진행되어 왔는데, 대부분은 일직선형(linear) 또는 굽힘형(bending) 구동이 주류를 이루고 있다. 이에 본 연구에서는 최근 생체적합성이 우수하여 인공근육재료로 주목받고 있는 Polypyrrole(PPy)을 금(Au) 전극 조건을 변화시키며 성장시켜 굽힘특성을 관찰하였다.

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Synthesis and Properties of a New Conjugated Polymer

박영진, *황선우, *장은혜, *채영준, *이상우, *김인태

*광운대 화학과 고분자연구실 *광운대 화학과*

A new conjugated polymer containing thiophene derivates in the main chain was successfully synthesized by Suzuki's cross coupling reaction. The resulting polymer was good soluble in organic solvents such as $CHCl_3$, CH_2Cl_2, THF and DMF. The structure of the resulting polymer was characterized by ^{1}H NMR, ^{13}C NMR, and FT-IR. The optical property and electronic property of the polymer was measured by UV-vis spectroscopy and PL, cyclovoltammetry, respectively. The polymer will be applied to LED as emitting materials.

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Synthesis and Properties of New Conducting Polymers for All Solid State Sensor

정연준, 허민, 신재호, 김인태

광운대 화학과

The conducting polymer is known as a material for improve performance of all solid state sensors. We synthesized new conducting copolymers containing hetero atom compounds with carbazole derivatives, benzobisthiazole and EDOT. The structure of the resulting polymers were characterized by ^{1}H-NMR, ^{13}C-NMR, and FT-IR. The optical properties and electronic properties of the resulting compounds were measured by UV-vis spectroscopy and cyclovoltammetry, respectively. The molecular weight of the copolymer was measured by GPC. Themal properties of the copolymer was investigated by TGA. The resulting polymers were applied to all solid state sensors.

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Photo Cross-Linkable TPD derivative Hole-Transport Material for Solution Processed Oled Light Emitting Diodes

한우택, 김인태

광운대 화학과

To achieve high-performance LEDs devices, enhanced recombination of electrons and holes in the emitting layer (EL). One of the approaches to solve this requirementist of abricate multilayer OLEDs by using hole-transporting layer(HTL), electron-transporting layer(ETL), andlight-emitting layer(EML) in device fabrication. However, the solution based preparation of multi-layer OLEDs introduces the problem that already coated layers tend to be at least partially dissolved by the solvent used to apply the next layer. A common method used to overcome this obstacle is to render the applied layer insoluble by cross-linking. For this purpose, TPD derivative bearing crosslingkable oxetane groups was synthesized. The new TPD derivative was characterized by ^{1}H-NMR, ^{13}C-NMR and FT-IR. The optical properties including UV absorption and photoluminescence of the TPD derivatives will be presented. The application of the new TPD derivative as hole transfer layer in LED will be discussed.

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Carbon ink 작업전극 사용하여 합성한 폴리피롤(PPy)의 액추에이터로서의 기계적 특성분석

권병국, 이현준

한국산업기술대 신소재공학과

전기활성고분자(Electro active polymer; EAP)는 전기에너지를 기계에너지로 직접 전환할 수 있는 물질로서 액츄에이터에 응용할 수 있다. 그 중에서도 폴리피롤(Polypyrrole; PPy)은 공기 중에서 작동성이 우수하며 전해중합을 통해 쉽게 얻을 수 있고 도핑물질 및 전극재료 등 합성조건에 따라 전기적, 물리적 특성을 쉽게 제어할 수 있다. 본 실험에서는 단량체로 Pyrrole 을 사용하였고, 전해액으로는 Polycarbonate 용액에 LiTFSI 를 용해하여 질소 purge 하여 사용하였으며, PVDF membrane 위에 carbon ink 를 Dip coating 하여 작업전극으로 사용하여 정 전류 전해중합법을 이용하여 폴리피롤을 합성 하였다. Dip coating 횟수 변화를 통해 carbon ink 두께에 변화를 준 sample 과 carbon ink 의 두께가 서로 같은 sample 에서 전류밀도 크기에 따른 PPy 의 액추에이터로서의 기계적 특성을 분석하므로서 carbon ink 의 두께와 두께에 따른 전기적 특성이 폴리피롤의 굽힘특성에 미치는 영향을 확인 하고자 하였다. 본 실험 결과 carbon ink 코팅횟수가 많은 sample 의 굽힘 특성이 상대적으로 더 좋았고 전류밀도를 크게 할수록 굽힘특성이 좋아 지는것을 볼 수 있으나, 어느 이상의 코팅횟수, 전류밀도에서 부터는 오히려 특성이 떨어지는것을 확인 할 수 있었다.

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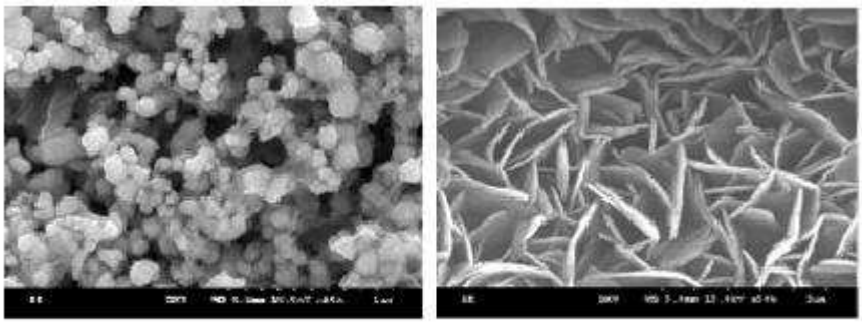
Fabrication of Superhydrophobic Surface with Controlling Growth of Nanoparticles

한문희

단국대 화학과

The chemical compositions and geometrical microstructure of surface are the key points to determine the wettability of surface. The study of super-hydrophobic surfaces have been focused to obtain a water contact angle greater than 150˚. In the nature, the phenomenon is the lotus-effect which can the found in the leaves of lotus. Nickel was deposited on metal surfaces with micro- and nano scale binary structure or micro-nano cones structure in the presence of crystal modifier. We report a simple method for fabricating nickel architecture on magnesium plate in aqueous solution by ethylene diamine as the modifying agent. In this experiment, the Mg plate was immersed in a mixed chemical solution(nickel and hydrazine and EDA) for 1hour and then immersed in stearic acid solution for 1hour. The surface morphology of modified Mg plate was analyzed with SEM, XRD, XPS and super-hydrophobic surface was determined by water contact angle measurement.



SEM images of deposited Ni metal on surface: (a) no additive applied (b) Ethylene diamine applied

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Conjugated Polymer Nanoparticles with Photoswitchable Multicolor Fluorescence for Bioimaging

정근수, *이용덕, *김세훈, 박종래

*서울대 재료공학부 *KIST 의과학연구센터*

We have developed a new type of fluorescent organic nanoparticles composed of densely integrated conjugated polymers and a diarylethene derivative. The nanoparticles were prepared via colloidal in situ polymerization in aqueous micelles containing highly concentrated photochromic molecules. By varying the monomer structure, the fluorescence color of the nanoparticles was readily tuned from visible to near-IR which is the spectra range favorable for bioimaging. Regardless of color, the fluorescence signal was stably and reversibly switched on and off by the irradiation of UV/visible light, through the effective nanoscopic energy transfer. Active intracellular internalization and reversible photoswitching of celluar fluorescence imaging demonstrate the potential of the rationally designed hybrid organic nanoparticles for advanced bioimaging applications.

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Synthesis and Properties of A emiconducting Polymer Induced Highly π-staking for Organic Thin-Film Transistors

장재완, *신민기, *고혜진, **김윤희, ***권순기

*경상대 고분자공학과 *경상대 고분자공학전공 **경상대 화학과 ***경상대 나노신소재공학부*

Organic thin film transistors (OTFTs) based on polymeric semiconductors as an active layer have attracted wide attention due to their potential use in low-cost, lightweight and flexible electronic devices. Recently, new polythiophenes and their analogues with various fused aromatic rings have been reported to show even higher carrier mobility. In this study, we designed a p-type thiophene based polymer containing alkoxy group with polycyclic aromatics to enhance wide π-conjugated area. We focused our attention on highly π-extended plane structure with four fused aromatic ring. PNDT was synthesized by oxidative cyclization and Yamamoto coupling reaction with high overall yields. The obtained PNDT polymer was characterized by elemental analysis, 1H-NMR, 13C-NMR, FT-IR, UV-absorption, photoluminescence (PL), and cyclicvoltammetry (CV) studies. The higher thermal stability of this polymer was determined using the thermogravimetric analysis (TGA) and differential scanning calorimeter (DSC) studies. OTFT device results using the polymer were also investigated. Detailed results will be presented in the presentation.

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

고용기, *진경식, 박삼대, 김진철, 김동민, 정정운, 노예철, 안병철, 권원상, 김경태, 김미희, 정성민, **최준만, ***권순기, ****김윤희, 이문호

*포항공과대 화학과 *포항공과대 포항가속기연구소 **포항공과대 화학관 ***경상대 나노신소재공학부 ****경상대 화학과*

We synthesized the three new dianhydrides, 1,4-bis (4'-t-butylphenyl) pyromellitic dianhydride (BBPD), 1,4-bis-(4'-trimethylsilylphenyl) pyromellitic dianhydride (BTPD), and 2,2'-bis(4''-tert-butylphenyl)-4,4',5,5'-biphenyltetracarboxylic dianhydride (BBBPAn) and a series of new organosoluble polyimides: BBPD-ODA, BBPD-MDA, BBPD-FDA, BTPD-FDA, and BBBPAn-FDA using the corresponding diamines: 4,4'-oxydianiline (ODA), 4,4'-methylenediamine(MDA), 4,4'-(hexafluoroisopropylidene)dianiline (6FDA) 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.

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Programmable Permanent Data Storage Devices based on Nanoscale Thin Films of a Thermally Stable Aromatic Polyimide

김동민

포항공과대 화학과

In this study, the synthesis of thermally and mechanically stable polyimide, (hexafluoroisopropylidenediphthalimide-4-hydroxytriphenylamine) (6F-HTPA PI) was successful and the nonvolatile memory devices based on a high performance polyimide, 6F-HTPA PI, were fabricated with a simple conventional solution coating process. The 6F-HTPA PI film exhibits excellent write-once-read-many-times (WORM) memory characteristics with and without polarity depending on the thickness and bottom electrode with a high ON/OFF current ratio of up to 10^6 and a long retention time in both ON and OFF states. These properties open up the possibility of the low-cost mass production of high density and very stable digital nonvolatile WORM memory devices.

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Synthesis and Electroluminescent Properties of New Triazole Derivatives with Naphthalene or Anthracene Cores

이남진, 이대희, *박영일, **이기호, *박종욱, 이지훈

*충주대 나노고분자공학과 *가톨릭대 화학과 **고등과학원 계산과학부*

The applications of π-conjugated organic materials to electronic devices have been expanded in various areas such as organic light-emitting diodes (OLEDs) for recent decades. In general, efficiencies and lifetimes of OLED devices were influenced by a good charge balance of electrons and holes. In particular, they were highly affected by other factors such as thermal stability, redox stability, and work functions of hole or electron transporting materials used in OLEDs. To further improve the performance of OLED, the development of efficient electron-transporting materials (ETMs) is still a major objective.In this study, a new electroluminescent materials based on triazole derivatives with naphthalene or anthracene cores were synthesized and their optical and thermal characteristics, and the characteristics of OLED device were experimentally and computationally examined.

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Fast Preparation of A Free-Standing Nacre-like Film by Solid-liquid Phase Separation

Sun Fangfang

부산대 나노융합기술학과

Fabrication of molecular level-controlled film allows producing optimally biocompatible films with high mechanical strength and homogeneous dispersity. However, the film fabrication with adequate thickness (sub-micro to millimeter) requires consecutive process with identical thermodynamic and kinetic conditions, which would need lengthy cost and time consumption, and potential limitation of suitable materials and already have been a bottleneck to be commercialized even though the technological advances has enlarged some essential productions in biological and gas sensing applications. In this article, we produced highly ordered and flexible nacre-like films from chitosan and hydroxyapatite. Dispersity, mechanical strength, and microstructure of the prepared film were characterized. Assessment of the film properties indicated that it exhibited homogenous dispersity and microporosity with satisfactory mechanical strength by use of innate interpolymeric repulsion in solution and the initial solidification temperature was quite crucial to characterize the dispersity and homogeneity of the organic/inorganic composites. The optimum ratio in the preparation of the highest flexible film was found to be 100 (w/w) %. This biocompatible nacre-like film through a simple and fast method might be directly applied to the industrial level production of bio-films for surgical appliances, wound dressings, space-filling implants as well as drug delivery systems.

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Design of pamam dendrimers modified with hydrophobic spacer and amino acids as a new nonviral gene delivery carrier

유광식, 최윤희, 최준식

충남대 생화학과

In this study, we prepared poly(amidoamine) derivatives that conjugated with 6-aminohexanoic acid and L-Arginine using HOBt/HBTU coupling method. 4th generation of poly(amidoamine) dendrimer was used because they displays relatively good transfection efficiency and low cytotoxicity than other generations. In our previous study, it was confirmed that L-arginine grafted poly(amidoamine) dendrimers displays much higher transfection efficiency while maintaining their cytotoxicity. 6-aminohexanoic acid was selected as a spacer molecule for enhance the hydrophobicity of dendrimers. 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, it is expected that this poly(amidoamine) derivatives could bind with plasmid DNA because they have primary amine groups on their peripheral end units.Synthesized PAMAM G4-Ahx-Arg was analyzed by 1H-NMR. It was confirmed that 98% of 6-aminohexanoic acid and 97% of L-arginine was conjugated to the surface of PAMAM G4, respectively. In agarose gel retardation study, PAMAM G4-Ahx-Arg formed polyplex formation at weight ratio of 8:1 (polymer : pDNA). In dynamic light scattering study, the mean diameter of polyplex was 177.5 ± 23.3nm. From the transfection assay results, PAMAM G4-Ahx-Arg showed much higher transfection ability compared with native PAMAM G4. Also, it was found that PAMAM G4-Ahx-Arg has very low cytotoxicity compared with PEI25KD in WST-1 assay results. From these results, it is thought that the combination of 6-aminohexanoic acid and L-arginine with poly(amidoamine) is beneficial for enhance their hydrophobicity while maintaining transfection ability and cytotoxicity.

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Stable Aqueous Dispersion of Reduced Graphene Nanosheets via Non-Covalent Functionalization with Conducting Polymers

조기영, *이태민, **김병수

*울산과학기술대 전기전자컴퓨터공학부 *울산과학기술대 나노생명화학공학부 **울산과학기술대 친환경에너지공학부*

Graphene, a single layer of two-dimensional carbon lattice, has recently attracted enormous interests with its remarkable electrical, thermal and mechanical properties. However, the problem is that it is hard to get pure graphene sheet in a scalable, and reproducible manner. The alternate solution for this problem is the chemical exfoliation by oxidizing the surface of graphene to make graphene oxide (GO) nanosheets. However, graphene oxides need an additional reduction process to recover the intrinsic properties of graphene. During this chemical reduction process, additive like ammonia is often mixed with GO solution to prevent the aggregation as well as to disperse the resulting reduced graphene oxide (RGO) nanosheets. Unlike common process, here in this study we employed the poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) as an additive during the reduction of GO. The resulting composite of RGO with PEDOT:PSS is well-dispersed in an aqueous solution without any noticeable aggregates for several months. We found that the strong pi–pi interactions between RGO nanosheets with PEDOT together with the presence of highly hydrophilic PSS group afford the necessary solubility and stability of RGO/PEDOT. Various methods were employed to characterize the composition and electrical properties of the RGO/PEDOT, including XPS, Raman, UV-vis, TGA, Elemental analysis, 4-point probe AFM, and SEM. We believe this finding, through further process optimization, will suggest the RGO/PEDOT hybrid film could become an attractive candidate for a large-scale flexible transparent conducting film for future optoelectronic devices.

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Chemiluminescent Nanoparticles for Hydrogen Peroxide and Glucose Imaging

이용덕, 김세훈

KIST 의과학연구센터

Water-dispersed all-in-one nanoparticles composed of densely integrated peroxyoxalate fuel and a cyanine dye are formulated to optimize the nanoscopic chemiluminescence reaction. It is demonstrated that the nanoformulation can generate bright chemiluminescence signal in response to external hydrogen peroxide that is biologically implicated with cell signaling and diseases. Successful imaging of endogenously overproduced hydrogen peroxide and indirect determination of glucose level in vivo/vitro with the chemiluminescent nanoprobes offer an opportunity for early diagnosis of diseases.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Hydrophobic modification of cationic dendrimer as a tool of nonviral vector system

최윤희, 유광식, 최준식

충남대 생화학과

The characteristic of the cationic polymer for gene delivery is affected by hydrophobicity. In this study, 6-aminohexanoic acid and ɣ-aminobutiric acid(GABA) were respectively conjugated to L-arginine grafted polyamidoamine dendrimer 4(PAMAM G4) as a spacer molecule. Comparatively high transfection efficiency of Arginine conjugated PAMAM was verified through our previous study. The 4th generation of PAMAM dendrimer was selected because of its relatively good transfection efficiency and low cytotoxicity compared to other generations. These synthesis progressed with HoBt/HBTU coupling reagents. As a spacer molecule, 6-aminohexanoic acid and ɣ-aminobutiric acid were used to increase hydrophobicity and to introduce the flexibility of the conjugated amino acids. It is also try to recognize effect of space molocule's lenth by comparing 6-aminohexanoic acid and ɣ-aminobutiric acid. These synthesized PAMAM conjugates were analyzed by 1H-NMR. Due to their peripheral primary amine, these compounds are capable of condensing with pDNA electrostatically. PAMAM-Ahx-Arg and PAMAM-GABA-Arg were examined the transfection efficiency by luciferase assay and protein assay. These compounds were also investigated cytotoxicity by WST-1 assay.

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Biocompatibility of Poly(propylene carbonate) Prepared from Copolymerization of Carbon Dioxide with Propylene Oxide

김진철, 이문호

포항공과대 화학과

In this study we investigated bacterial and cell adhesion to poly(propylene carbonate) (PPC) films, synthesized by copolymerization of carbon dioxide (a global warming chemical) with propylene oxide. We also assessed the biocompatibility and biodegradability of the films in vivo, and their oxidative degradation in vitro. It was found that there was adhesion of bacteria to the smooth, hydrophobic PPC surface after 4 h incubation; Pseudomonas aeruginosa and Enterococcus faecalis had the highest levels of adhesion, Escherichia coli and Staphylococcus aureus had the lowest levels, and Staphylococcus epidermidis was intermediate. In contrast there was no adhesion of human cells (cell line HEp-2) to the PPC films, due to the hydrophobicity and dimensional instability of the surface. On the other hand, the PPC films exhibited good biocompatibility in the mouse subcutaneous environment. Moreover, surprisingly the PPC films were found to degrade in the mouse subcutaneous environment. This is the first time that PPC can undergo surface erosion biodegradation in vivo. The observed biodegradability of PPC may have resulted from enzymatic hydrolysis and oxidative degradation processes. In contrast, the PPC films showed resistance to oxidative degradation in vitro. Overall, PPC reveals high affinity to bioorganisms and furthermore good biodegradability.

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Biocompatible Brush Polymers Bearing Various Glycine Derivatives with Self-Assembled Structures

정정운, 박삼대, 김진철, 김동민, 안병철, 권원상, 김경태, 고용기, 정성민, *최준만, 이문호

*포항공과대 화학과 *포항공과대 화학관*

We designed polymers containing the glycine derivatives methylglycine, dimethylglycine, and acetylglycine, which form films with significant biocompatibility. These functional groups were incorporated onto the ends of the long alkyl bristles of a PECH-based brush polymer to form the polymers PMUTE, PDUTE, and PAUTE. The thin films of each of these brush polymers were investigated to determine their morphological structure, hydrophilicity, hydrophobicity, water sorption, blood compatibility, bacterial adherence, cell adhesion, and biocompatibility in mice. The thin films of all three brush polymers were found to contain a multi-bilayer structure supported by the laterally ordered bristles as well as hydrogen bonding of the glycine derivatives at the bristle ends, which can provide surfaces enriched with functional groups. These structural differences result in different water sorption behaviors of the films of the brush polymers

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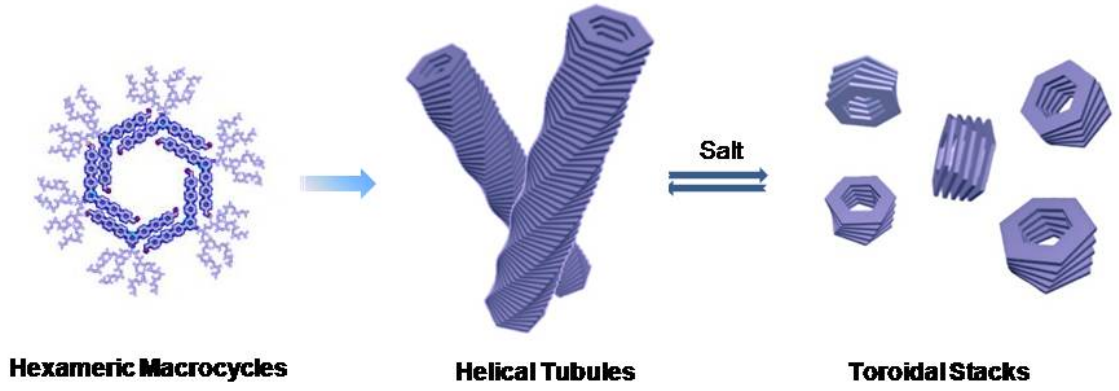
Dynamic Tubules from Helical Stacking of Noncovalent Macrocycles

강성균, *이명수

*서울대 화학부 *서울대 화학과*

We synthesized a laterally-grafted bent rod amphiphile consisting of a meta-linked aromatic segment and an oligoether dendron side group. It self-assembles into an elongated tubular structure with an internal diameter of ~3 nm through π-π stacking and electrostatic interactions. Notably, addition of a certain amount of silver dodecylsulfate as a hydrophobic guest triggers the cylinderical aggregates to dissociate into discrete toroidal stacks. The formation of the cylindrical aggregates and the toroidal structures were confirmed by TEM and AFM experiments performed in aqueous solutions.



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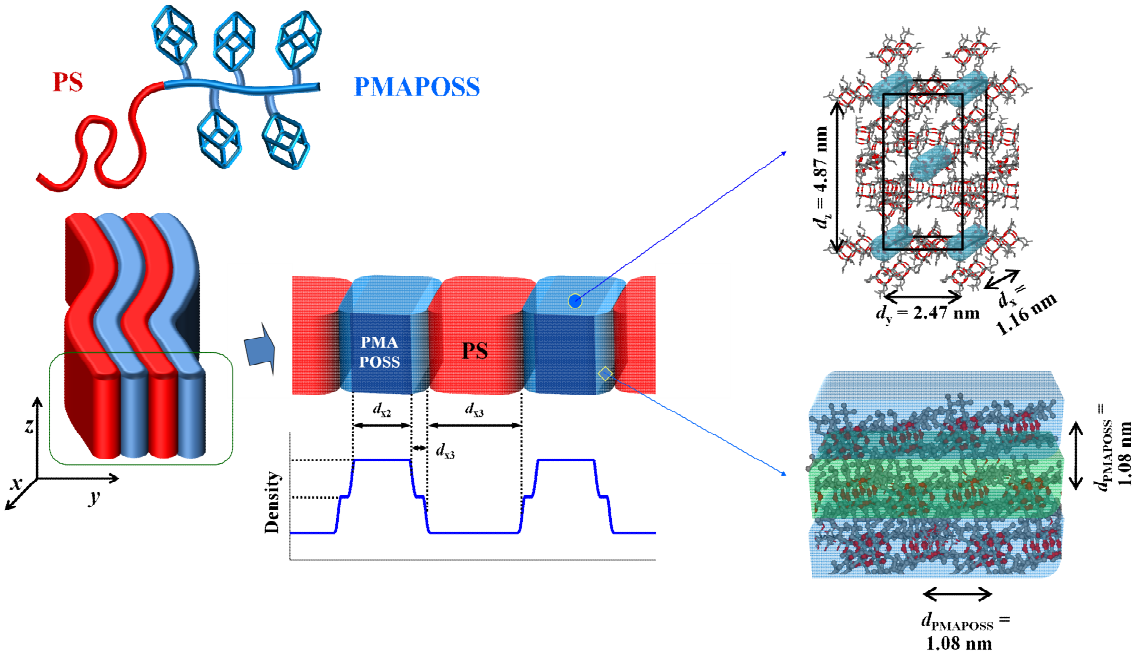
Hierarchical Structures in Nanoscale Thin Films of Lamellar-forming Poly(styrene-b-methacrylate grafted with POSS)

안병철, *Hirai Tomoyasu, 노예철, 정성민, 김경태, 정정운, 김미희, 김동민, 권원상, 고용기, 박삼대, 김진철, **최준만, *Hayakawa Teruaki, ***Gopalan Padma, 이문호

*포항공과대 화학과 *Tokyo Institute of Technology, JAPAN **포항공과대 화학관 ***Univ. of Wisconsin, USA*

An interesting organic-inorganic diblock copolymer, poly(styrene-b-methacrylate grafted with polyhedral oligomeric silsesquioxane) (PS-b-PMAPOSS). The morphological structures in nanoscale thin films of PS-b-PMAPOSS were investigated in detail by grazing incidence X-ray scattering (GIXS). GIXS formulas based on structural models were derived for the quantitative analysis of scattering data. The quantitative 2D GIXS analysis found that the diblock copolymer molecules in the thin films undergo phase separation into PS and PMAPOSS domains, which generates a lamellar structure. Surprisingly, this lamellar structure is completely oriented in the out-of-plane of the film and is stable up to the degradation temperature. The PMAPOSS layers in the lamellar structure were found to consist of two sub-layers, namely a densely ordered layer composed of vertically oriented orthorhombic crystals and a less ordered layer that consists of molecularly stacked layers that are oriented vertically.



대 한 화 학 회
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Synchrotron Grazing Incidence Wide-Angle X-ray Scattering Study on Molecular Aggregation Structures of Fully-aromatic and Semialiphatic Polyimide Films

김경태, *Junji Wakita, 안병철, 박삼대, 김진철, 김동민, 정정운, 권원상, 고용기, 정성민, 최준만, 이문호, *Shinji Ando

*포항공과대 화학과 *Tokyo Institute of Technology*

The intermolecular aggregation structures of fully aromatic polyimides (Ar-PIs) prepared from pyromillitic dianhydride and those of semialiphatic polyimides (Al-PIs) from 4,4'-diaminocyclohexylmethane were characterized by grazing incidence wide-angle X-ray scattering (GIWAXS) technique. The aggregation structures of Ar- and Al-PI thin films formed on Si substrates were identified as a mixture of ordered and amorphous domains. For Ar-PIs with glass transition temperatures (Tg) higher than the imidization temperature (Ti), the aggregation structures are significantly influenced by the three-dimensional structures of the PI chain. Rodlike molecular structures with high planarity are prerequisites for the growth of ordered domains of Ar-PIs, whereas an Ar-PI having a bent and nonplanar structure exhibits the highest amorphous characteristics. In addition, the bulky -CF3 groups in the diamine moiety increase the interchain distance in the ordered domains. For Al-PIs with Tgs lower than Ti, the degree of interchain ordering was higher than those of Ar-PIs, but was decreased significantly by decreasing Tgs. This is due to the vigorous motion of PI chains during thermal imidization.

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Effect of C_{60} Fullerene on the duplex formation of i-motif DNA in solution using Synchrotron X-ray scattering

김미희, *진경식, 안병철, 정성민, 박삼대, 김진철, **김동민, 정정운, 권원상, 김경태, 고용기, 최준만, 이문호

*포항공과대 화학과 *포항공과대 포항가속기연구소 **부산대 화학과*

The structural effects of fullerene on i-motif DNA were investigated by characterizing the structures of fullerene-free and fullerene-bound i-motif DNA, in the presence of cDNA in solutions of varying pH, using circular dichroism and synchrotron small-angle X-ray scattering. To facilitate a direct structural comparision between the i-motif and duplex structures in response to pH stimulus, we developed atomic scale structural models for the duplex and i-motif DNA structures, and for the C60/i-motif DNA hybrid associated with the cDNA strand, assuming that the DNA strands are present in an ideal right-handed helical conformation. We found that fullerene shifted the pH-induced conformational transition between the i-motif and the duplex structure, possibly due to the hydrophobic interactions between the terminal fullerenes and an internal TAA loops in the DNA strand. The hybrid structure showed a dramatic reduction in cyclic hysteresis.

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Prediction of Structure and Mechanical Properties of Crosslinked Epoxy Resin by Molecular Dynamics Simulation

김혜미

LG화학기술연구원

Molecular dynamics (MD) simulations were used to predict the properties of diglycidyl ether of bisphenol A (DGEBA) crosslinked with curing agent isophorone diamine (IPD). This polymer is a commercially important epoxy resin and a candidate for application in nanocomposites. We developed the atomistic models of crosslinked epoxy resin using iterative MD/MM (molecular mechanics) procedure where bond formation and MD/MM relaxation steps are repeated until degree of crosslinking reaches experimental value. Density, bulk modulus, and glass transition temperature of the epoxy resin system are predicted. The simulated results compared reasonably with experimental data available.

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Electrical Memory Characteristics of a Poly(1,6-heptadiyne) With Carbazole Moieties

박삼대, 김동민, 김진철, 김경태, 권원상, 고용기, 장태현, 이문호

포항공과대 화학과

Poly[bis(9H-carbazole-9-ethyl)dipropargylmalonate] (PCzDPM) is a novel p-conjugated polymer bearing carbazole moieties that has been synthesized by the polymerization of bis(9H-carbazole-9-ethyl)dipropargylmalonate with the aid of molybdenum chloride solution as the catalyst. This polymer is thermally stable up to 255 °C under a nitrogen atmosphere and 230 °C in air ambient; its glass transition temperature is 147 or 128 °C, depending on the polymer chain conformation (helical or planar structure). The charge-transport characteristics of PCzDPM in nanometer-scaled thin films were studied as functions of temperature and film thickness. PCzDPM films with a thickness of 15−30 nm were found to exhibit very stable dynamic random access memory (DRAM) characteristics without polarity. Furthermore, the polymer films retain DRAM characteristics up to 180°C. The ON-state current is dominated by Ohmic conduction and the OFF-state current appears to undergo a transition from Ohmic to space charge limited conduction with a shallow-trap distribution. The ON/OFF switching of the devices is mainly governed by filament formation. The filament formation mechanism for the switching process is supported by the metallic properties of the PCzDPM film, which result in the temperature dependence of the ON-state current. In addition, the structure of this conjugated polymer was found to vary with its thermal history; this change in structure can affect filament formation in the polymer film.

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Temperature Sensitive Polypeptide for drug delivery system

장지혜, 주민경, *윤은정, 정병문

*이화여대 화학나노과학과 *이화여대 바이오융합과학과*

Polymers that form hydrogels in response to stimuli, like temperature, pH, ionic factors, chemical agents, have important potential for use as clinical area such as injectable depot drug delivery systems and tissue engineering. In this study, we investigated the pH- and temperature responsive hydrogel system for sustained releasing by electrostatic interaction.

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Intelligent Hydrogels from Peptide Amphiphiles

박일수, 이명수

서울대 화학과

We have found that hydrogel is transformed into a fluid solution by an addition of a C_{60}. To solve this phenomenon, we have synthesized some peptides which are tryptophan-rich and have PEO short chains. These peptides are self-assembled into fiber-like structures. When the concentration increase, the fibers are entangled together to form a hydrogel. However, the hydrogel is transformed to fluid solution as an addition of a hydrophobic C_{60}. The indole in which is the functional group of a tryptophan has an interaction with a C_{60}. For the existence of an interaction, these nano-fibers can complex with a C_{60}. It causes that the nano-fiber contained C_{60} is snapped and a hydrogel transform into a fluid solution. We expect that these peptides can be used as a bio-active nano-fiber which can response to a C_{60}.

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A "Green" Catalytic Polymerization of Anthracene by Friedel–Crafts Alkylation within the Nano-channels of controllable FeSBA-15 Mesoporous

김정훈, *Chokkalingam Anand, 유정목, *Ajayan Vinu, 김은경

*연세대 화학공학과 *National Institute for Materials Science, Japan*

Highly ordered mesoporous silica was used as a template for catalytic polymerization of anthracene. The Fe(III) incorporated mesoporous silica, FeSBA-15, was synthesized by changing of iron content and synthesis temperature for various iron contents and pore diameter. The iron incorporated mesoporous catalysts were used as an oxidative nano-reactor in catalytic reactions to afford highly fluorescent poly(methylene anthracene)s (PMAn), of which structure were controlled by the pore size and shape of the template. The polymerization by Friedel–Crafts alkylation showed high yield and higher Mw even in use of small amount of catalyst compared to homogeneous catalytic polymerization of anthracene. The pore size of the reactor was critical to the emission properties of the resultant polymers. The excimer emission was strong in PMAn synthesized from a smaller pore reactor, opening new catalytic polymeric reactions not only limited to Friedel-Crafts type reaction. Herein we report the effective catalytic polymerization of anthracene using iron incorporated highly ordered mesoporous silica with controllable nano-sized reactor channel.

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Size Selective Separation of Giant Unilamellar Vesicles Using a Microfluidic chip

허유희, *신관우, **이기라

*서강대 화학과 *서강대 화학과 및 바이오융합과정 **충북대 공업화학과*

Giant unilamellar vesicle (GUVs), consisting of single phospholipid membranes with diameters greater than 10 μm, are excellent biological models for dynamics and physical properties of many biological phenomena. Among various preparation methods of GUV, electroformation method, where external electric field is applied to lipid films deposited on an electrode, is commonly used to produce GUVs. In this work, we prepared 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) to synthesize the GUVs. However, it is very difficult to control the homogeneously sized GUVs, often showing a broad distribution in the vesicle diameters. Although the conventional electroformation for the GUV production seems to be inevitable, we designed a microfluidic chip, which could separate the smaller GUVs with diameter less than 10 μm. After the filtration, we could obtain GUV solution with a narrower distribution in their GUV sizes. In this presentation, we will present the design of the microfluidic chip and the performance of size-selectivities. The number of selection slits, the flow rate, and the number of filtration cycles was varied to optimize the separation efficiency.

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Thermogelling behavior of PAL-PLX-PAL

문효정, *박민희, **박수현, 정병문

*이화여대 화학나노과학과 *이화여대 나노과학부 **이화여대 바이오융합과학과*

The aqueous solution of PAL-PLX-PAL in a concentration range of 3~15 wt% underwent sol-to-gel transition as the temperature increased from 10 to 50 ^{o}C. The sol-to-gel transition temperature could be controlled by varying the molecular weight of each block, ratio of Ala to Leu. 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 PAL-PLX-PAL was degradable by elastase, chymotrypsin, cathepsinB, cathepsinC, and MMP-2 in vitro. The in vitro release study of BSA-FITC from the gel was performed. and the in vivo release studies using SD rat revealed that the plasma concentration of BSA-FITC was maintained for 2weeks.

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Self-assembled Semiconducting Monolayer prepared with Triethoxysilane-functionalized X-shaped Conjugated Molecule

이주빈, 하재승, 이태완, 김경환, 최동훈

고려대 화학과

Recently, we reported very interesting semiconducting properties of anthracene based conjugated molecules, investigated in thin film transistors. The anthracene moieties demonstrated quite unique molecular aggregation and strong intermolecular interaction in the solid state. From this motif, we prepared triethoxysilane bearing the corresponding semiconducting moiety as a precursor molecule for elaborating self-assembled monolayer (SAM) on the hydroxyl functionalized substrate. The absorption and emission properties of SAM were compared with those of solution and bulk films. With the deposition condition, the density of semiconducting molecules and the packing structures were investigated using atomic force microscope and laser scanning fluorescence microscope.

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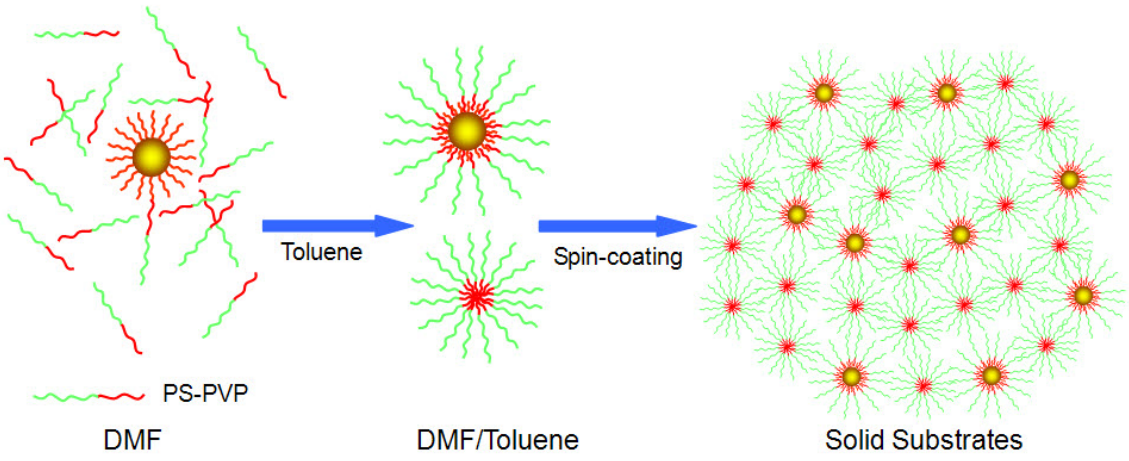
Solvent-induced Self-assembly of Polymer-grafted Au NPs/block Copolymers and Their Spin-coated Composite Nanofilms

Dongxiang Li, *이지용, 김동하

*이화여대 화학나노과학과 *이화여대 화학과*

Gold nanofilms have displayed significant potential in multidisciplinary fields. In this work, the cooperative self-assembly of poly(4-vinylpyridine) grafted gold nanoparticles (Au NPs) and poly(4-vinylpridine)-b-polystyrene block copolymers (BCPs) was performed by introducing a selective solvent to the solution. The assembled mixtures were spin-coated onto solid substrates to fabricate composite gold nanofilms consisting of Au NPs hybridized with the BCPs and independent BCPs micelles. The obtained gold nanofilms displayed different morphology changes in the vapor annealing of selective solvents due to the adsorption and dissolution of solvent molecules in the nanofilms. The interaction between vapor and polymer segments in the nanofilms might have a potential in the vapor/organic sensing based on the large accommodation space inside the polymer domains.



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Heavy-Atomic Construction of Photosensitizer Nanoparticles for Enhanced Photodynamic Therapy of Cancer

신지영, *이용덕, *김세훈

*경희대 나노의약생명과학과 *KIST 의과학연구센터*

We report a photophysically motivated nanoformulation approach to develop an advanced nanomedicine platform for photodynamic therapy. Our strategy is based on the utilization of the nanoscopic heavy-atom effect on the nanoparticle-encapsulated photosensitizer that can enhance singlet oxygen generation by the promoted intersystem crossing. Furthermore, the encapsulation in Pluronic-based nanoparticles facilitates the internalization of photosensitizers into live cancer cells through the enhanced endocytosis. Overall, the beneficial features offer an optimal nanoplatform to improve the efficacy of photodynamic therapy.In this presentation, we describe in detail the construction of highly iodinated Pluronic nanoparticles with biocompatible constituents and spectroscopic studies on their singlet oxygen generation capabilities. By experiments for imaging and phototoxicity evaluation with human breast cancer cells, we demonstrate that our photophysically engineered nanomedicine has great potential for photodynamic therapy of cancer, by accelerating the light-triggered induction of apoptosis.

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Conducting Pattern of CNT with using Ink-Jet Printing Method

김한수, *신관우, 이병노

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

Compare to lithographic process, the ink-jet printing process with carbon nanotube (CNT) is an attractive approach for producing electrical circuit with low production costs and flexibility for the substrates such as papers, OHP films, or membranes. It is environment-friendly as well as economical, because the ink-jet printing is drop-on-demand (DOD) printing process, no waste of ink and substrates. Although there are some publications to print CNT inks with a ink-jet printer, the conductivities of printed patterns are not high even with the pattern of 90 times overprint probably due to very low concentration of CNT and/or unsmooth printing. In this study, we prepared a series of formulated CNT-ink from CNT dispersion liquid for the ink-jet head of piezo type, and the materials printed with them give lower resistance values of (less than or up to) 200Ω/sq on the paper that is measured after two days : it could be acceptable for producing a simple conducting circuit. The conductivity of CNT solution could be improved by the addition of other conducting materials such as PEDOT:PSS and/or poly-aniline, which are currently under investigation. The differences between piezo and thermal head are also investigated.

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Organic Single-crystal Field-Effect Transistors Fabricated with 2-Dimensional Conjugated Molecules bearing Thiophenyl Peripheral Arms

배숙영, 조소영, 김경환, 이태완, 최동훈

고려대 화학과

In the solid state of organic semiconductors, the intrinsic carrier mobility depends critically on the degree of molecular orientation and on the extent of the intermolecular interaction. In this study, 2-dimensional conjugated molecules were synthesized. In the exploration of the application as organic semiconductors in organic field effect transistor (OFET) is an important component for developing future flexible displays. Introduction of thiophene-based peripheral moieties into an anthracene core improve the solubility in organic solvent for facilitating the solution device fabrication. They showed intriguing microscopic self-organization of molecules inducing the anisotropic alignment. We investigated the field effect transistor properties of solid films and single crystals using the molecules we synthesized recently.

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Low-bandgap X-shaped Anthracene Derivative bearing 4-(thiophen-2-yl)benzo[c][1,2,5]thiadiazole Peripheral Groups

허정아, 김경환, 이태완, 신지철, 최동훈

고려대 화학과

Semiconducting materials based on π-conjugated organic molecules have been extensively investigated for applications in variety of optoelectronic devices. In the study, we synthesized low-bandgap X-shaped molecules and characterized their properties. We present here the synthesis of anthracene derivatives containing 4-(thiophen-2-yl)benzo[c][1,2,5]thiadiazole as peripheral groups. In the new compound which contains the 2,1,3-benzothiadiazole, it is well established that intramolecular charge transfer from electron-rich to electron-deficient moieties lowers the band-gap, which is desirable for organic photovoltaic cell. These molecules display a p-type semiconducting behavior and their electrical properties are investigated in detail.

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Photocontrolled Organic Thin Film Transistors Using Soluble Anthracene-based Conjugated Molecules

김윤선, Hoang Mai Ha, 이태완, 김경환, 최동훈

고려대 화학과

Recently, we reported very interesting semiconducting properties of anthracene based conjugated molecules bearing thiophenyl peripheral groups. The anthracene-based molecules showed very intriguing J-aggregation behavior in the solid state evidenced by absorption and emission spectroscopy. Conjugated organic molecules and polymers have also been used for light-emitting diodes and photovoltaic cells because of their excellent photoexcitation property. The control of the charge concentration in the OTFTs through the gate bias and the photoinduced enhancement of charge carriers under irradiation of excitation light can lead to investigate the potential of phototransistors and corresponding photocontrolled memory devices. In this study, we fabricated TFT devices using anthracene-based conjugated molecules bearing thiophenyl peripheral groups. And we investigated the photosensitivity of TFT devices under dark and illumination condition and effect of light irradiation on the device properties in detail.

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장소: 대구엑스코
발표코드: **POLY.P-66**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

X-Ray Scattering Studies on Poly(3-hexylthiophene) Nanoporous Structure Using a Block Copolymer Template System

노예철, *Ayumi Takahashi, *Tomoya Higashihara, 안병철, 정성민, 김경태, 정정운, 박삼대, 김진철, 김동민, 권원상, 김미희, 고용기, **최준만, 이문호, *Mitsuru Ueda

*포항공과대 화학과 *Tokyo Institute of Technology **포항공과대 화학관*

Regioregular poly (3-hexylthiophene)s (P3HT-NH_2) and sulfo-chain-end- functionalized polystyrene (PS-SO_3H) have been prepared and block copolymers via ionic interaction, (P3HT-NH_3+)-b-(PS-SO_3-)s, were successfully synthesized, simply by blending P3HT-NH_2 with PS-SO_3H in toluene. The self-assembly behavior of the (P3HT-NH_3+)-b-(PS-SO_3-) thin film was observed grazing incidence X-ray scattering (GIXS) analysis. By exploiting the pH-sensitive ionic interaction, the PS-SO_3- domains were selectively etched with ethyl acetate/triethylamine, cleaving the ionic interaction between P3HT-NH_3+ and PS-SO_3- segments, to obtain the target nanoporous P3HT-NH_2 films. The porosity of the films was confirmed by GIXS analyses, AFM and TEM.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Size-selective cellular uptake mechanism and efficiency of nano- and microparticles protected by cell penetrating peptides

김희석, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

Fluorescent dye labeled various size silica particles consisting of nano- microparticles (from 30 nm to 1 μm) were synthesized by the Stöber method. In order to improve the cellular uptake efficiency into the cytoplasm without physical disruptions of the cell membrane, we have modified silica particles by HIV-1 trans-activator factor (TAT) protein which is known as very efficient cell-penetrating peptide (CPP). Depending on the size, shape of the carries, and the composition of the protecting molecules, the penetrating mechanism and efficiency into plasma cell membranes and membranes of the target intracellular compartments (i.e. nucleus) are widely varied, yet not fully understood. To investigate the delivery mechanism and efficiency of cellular uptake, we compared the fluorescence intensities inside cell by Flow cytometry analysis. Although flow cytometry analysis indicated that most CPP-coted particles can penetrate into the cell membrane easily, the larger particles (>200 nm, ≦800 nm) showed much stronger fluorescent intensity than smaller particles (≦200 nm). In case of smaller particles, CPP modified particle have higher fluorescence intensity than unmodified ones. Furthermore, we will present the size effects of 30 nm and 1 μm-particle for internalization process.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Microwave-induced Crack Healing in Perfluorocyclobutane-type polymers

유미란, 조성열, 정찬문

연세대 화학과

The object of this study is to develop an intelligent polymeric material in which cracks can be readily healed by microwave irradiation. The reaction by microwave irradiation has advantages such as better process control, faster curing times, and higher yields compared with the reaction by conventional heating. Perfluorocyclobutane (PFCB)-containing polymers have been studied as a unique class of fluoropolymers having excellent properties such as low dielectric constant, good thermal stability, high Tg, and optical transparency. In this work, the potential of PFCB polymers as a mendable material was investigated by means of microwave irradiation.The crack-healing ability of the polymers was investigated by FT-IR. The crack healing in the polymers was successfully demonstrated by the measurement of flexural strength of the polymer specimens before and after healing.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

In situ poly(urea-formaldehyde) microencapsulation of photoreactive healing agents

조예현, 조성열, 정찬문

연세대 화학과

The preparation of microcapsules for application in the fabrication of self-healing composites has been paid more attention. The microcapsules must possess sufficient strength to remain intact during processing of the host polymer, yet rupture when the polymer is damaged. High bond strength to the host polymer combined with a moderate strength microcapsule shell are required. To provide long shelf-life the capsules must be impervious to leakage and diffusion of the encapsulated healing agent for considerable time. A series of microcapsules were prepared by in situ polymerization method with poly(urea-formaldehyde) as a shell material and cinnamate-containing compounds as core materials. Microcapsules are composed of a smooth inner shell and, a rough, porous outer surface of agglomerated urea-formaldehyde nanoparticles. The chemical structure of microcapsule was characterized using infrared spectroscopy. The size, size distribution, morphology, and wall thickness were controlled by processing parameters such as agitation rate and core-shell ratio, and they were characterized by optical microscopy and scanning electron microscopy (SEM). The microcapsule size and wall thickness decreased when agitation rate increased.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Cinnamate-type Siloxanes as Photochemical Crack Healing Agents

송영규, 조성열, 정찬문

연세대 화학과

Polymeric materials are used in a variety of applications, but they are susceptible to damage induced by various physical and chemical factors. This results in microcrack formation and propagation, ultimately leading to significant reduction in mechanical performance and other desired properties of the materials. Recently, much attention has been paid to crack healing in polymeric matrixes. In this work cinnamate-containing siloxanes were synthesized as healing agents and their applicability to crack healing was investigated.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Influence of H_2O_2 on thermal and weathering degradation of poly(propylenecarbonate)

KodiyanVarghese Jobi, 박지혜, 이분열

아주대 분자과학기술학과

High molecular-weight poly(propylene carbonate) (PPC) can remain intact upon storage in ambient air or in water for 8 months once the catalyst is completely removed. Catalyst-free pure PPC is also thermally stable below 180^0C. At 200^0C, degradation occurs, mainly due to attack of the chain-ended hydroxyl group onto a carbonate linkage, through which the molecular weight distribution is broadened by simultaneous formation of low and high molecular weight fractions. Incomplete removal of hydrogen peroxide generated during the catalyst preparation results in a prepared polymer that contains a substantial amount of polymer chains grown biaxially from hydrogen peroxide, which gives rise to more severe thermal degradation. Experiments conducted in a weathering chamber at high temperature (63^0C) and high humidity (50%) revealed another degradation process involving chain scission through an attack of water molecules onto the carbonate linkage, which progressively and temporally lowers molecular weight.

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장소: 대구엑스코
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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

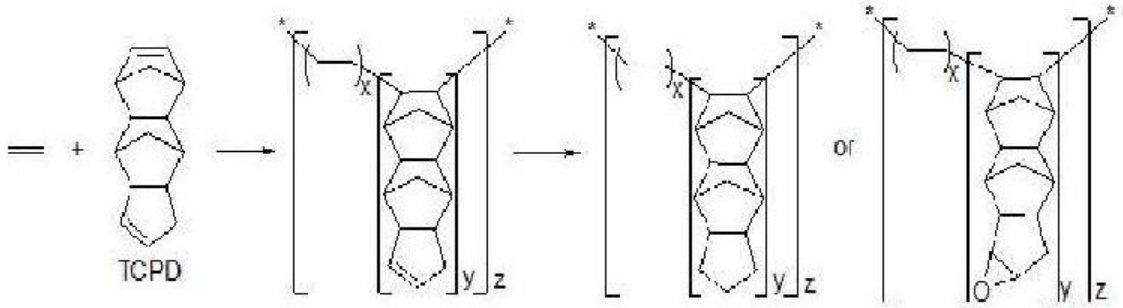
Copolymerization of Ethylene and Tricyclopentadiene

박형철, 이분열

아주대 분자과학기술학과

Copolymerizations of ethylene and tricyclopentadiene (TCPD) are realized without cross-linking with a high activity (3 - 18 x10^6 g/molZr·h) using a catalytic system of $[Ph_2C(Flu)(Cp)]ZrCl_2$/ MAO. The monomer reactivity ratios, $r_{ethylene}$ and r_{TCPD}, determined through the Fineman-Ross plot, were 6.4 and 0.044, respectively, indicating that TCPD insertion is unfavorable with the successive TCPD insertions being negligibly allowed. A significant higher Tg is attained than those observed for other reported cycloolefin copolymers at the same cycloolefin content. A high Tg of 214 ℃ is attainable at a TCPD content of 41 mol%. The remaining double bond can be quantitatively converted to an epoxide group or hydrogenated to saturated hydrocarbon.

Figure 1. Epoxidation and hydrogenation of ethylene/TCPD copolymers.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **POLY.P-73**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Immortal CO_2/Propylene Oxide Copolymerization and Architecture of Various Block Copolymers

Anish Cyriac, 이분열

아주대 분자과학기술학과

A highly active and relatively cheap catalyst for CO_2/propylene oxide (PO) copolymerization is developed (TOF 15000 h^{-1}). It was revealed that the high activity of these kind of complexes, due to an unusual binding mode of a Cobalt(III) complex prepared from a Salen-type ligand tethered by four quaternary ammonium salts. This catalyst preserves an excellent catalytic performance even in the presence of a large amount of protic compounds which enables us to efficiently perform "immortal polymerization" in CO_2/propylene oxide copolymerization. Precise control of molecular weight is achieved by feeding various protic compounds such as adipic acid, which resulted in the formation of low molecular weight poly(propylene carbonate)-diol (PPC-diol). Using PPC-diol, we have demonstrated polyurethane formation. Various three armed and star shaped polymeric structures made by simply feeding three armed and four armed carboxylic acids. From the data set (adipic acid 50-600 equivalent) of the absolute Mn (y) and the GPC-measured Mn (x) fit almost perfectly to an equation of $y = 0.255x^{1.09}$ ($r^2 = 0.997$). From this fitting the Mark-Houwink parameters of PPC, "K" and "α" are calculated to be 0.063 mL/g and 0.61, respectively. By feeding bulk polymer contains OH or COOH in immortal polymerization, we have demonstrated block and graft copolymerization. Additional melting region with slightly higher glass transition temperature is introduced by feeding PE-monoalcohol or PEG. A sheet prepared from PPC-*block*-PEG of 8.3 w% PEG unit is not as brittle as that of PPC itself. It is flexible and stretchable as the conventional PE film. A sheet prepared from PPC-*block*-PS of 11 w% PS unit is translucent and tougher than PPC itself.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of new PFDTBT based conjugated polymers for organic solar cells

김지훈, 황도훈, *신원석, *윤성철, *문상진, *이창진

*부산대 화학과 *한국화학연구원*

A series of electroactive and photoactive conjugated copolymers based on Fluorene and Benzothiadiazole, Perylene units polymers were synthesized using a Suzuki coupling polymerization by controlling the monomer ratios. The ratio of Perylene in copolymers decreased the peak and onset absorption of the copolymers moved to longer wavelength region so that band gap energies became smaller. The maximum UV absorption of the polymer films ranged in 489~550 nm and the optical band gap energies 1.94~1.85eV. Energy levels of the highest occupied molecular orbital (HOMO) were also determined by cyclic voltametry (CV). The determined HOMO energy level of the copolymers was around -5.45 eV. Photovoltaic devices were fabricated using the copolymers as the p-type donor and C60-PCBM or C70-PCBM as the electron acceptors. The device using Poly(F8T2BT10P) and C70-PCBM showed best device performance among the fabricated devices. The open circuit voltage, short circuit current, fill factor and the maximum power conversion efficiency of the best device were 0.74 V, 7.19 mA/cm2 ,0.40 and 2.15%, respectively.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Photo-crosslinkable Arylamine Monomer for Conjugated Aromatic Hole-Injection Material in OLED

송무곤, 최홍진, *박이순

*경북대 응용화학과 *경북대 고분자공학과*

A new arylamine monomer with photo-crosslinkable styrylpyridinyl moiety of conjugated polyarylamine for OLED hole injection material was synthesized through two synthetic routes, BOC-amine protection/deprotection and nitro group reduction methods. Both synthetic routes yielded practically pure amine product by standard aqueous workup and crystallization in reasonable yield. Their reaction efficiencies were comparatively studied in views of practicality and reaction scale. Also, the key compound of photo-crosslinker, 4-[2-(2-pyridinyl)ethenyl]phenol was reinvestigated, and the reproducible and optimized preparation condition was presented.

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장소: 대구엑스코
발표코드: **IND.P-1**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Preparation and Identification of Dicyclopentadiene Derived Alkyl compounds

박수열, *고은주, **최진일, ***정근우

*한국화학연구원 색소화학연구팀 *한국화학연구원 그린화학연구단 **한국화학연구원 에너지소재 ***한국화학연구원 응용화학연구단*

Dicyclopentadiene(DCPD) is a byproduct of C5 streams in oil refineries. The one equivalent of DCPD is readily decomposed into two equivalent of cyclopentadiene(CPD) at 180-200℃ with highly purity DCPD. In general, the DCPD can be widely application in several polymers such as ethylene, propylene, unsaturated polymer, olefin and epoxy resins. In our experiments, the DCPD derivatives were prepared from the reaction of a various alkyl compounds, i.e. O-alkyl, alkylhalide, O-alkylhalide and N-alkylation with a dicyclopentadiene at molar rations of 1:1 and 2:1. The optimal reaction conditions are as follows: toluene and O-dichlorobenzene as a solvents or not, temperature 110-160℃ and 5-24 hours reaction with yields of 30-70%. The GC, MS and FTIR were used to monitor and identify.

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

The Synthesis of New Coumarins Based Extended Donor-Acceptor Chromophores

안경룡, *신종일, **신승림, ***박수열, ****이상오, 박균하, *전근

*충남대 화학과 *한국화학연구원 신화학연구단 **한국화학연구원 염료염색가공연구센터 ***한국화학연구원 색소화학연구팀 ****충남대*

The synthetic route to coumarin system is well established and one approach of particular interest leads to the intermediate 7-diethylamino-3-formycoumarin. The Knoevenagel type condensation of this aldehyde with active methylene compounds can then lead to a coumarin systems with extended conjugation. A combination of the N,N-diethylaminocoumarine donor with a wide range of acceptor groups of varying electron withdrawing strength should permit the synthesis of a series of extended coumarin chromophores with absorption maxima ranging from 400 to 600 nm in a fluorescent properties some cases. Their use as laser dye, energy converters in the light collecting systems and as colorants for plastics was also noted.

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

ABSORPTION OF SULFUR DIOXIDE IN TASK SPECIFIC IONIC LIQUIDS CONTAINING SO2-PHILIC GROUPS ON THE CATION

홍성윤, 김대원, 김진형, 정민석, 김훈식

경희대 화학과

Fossil fuel burning power plant is one of major producers of sulfur dioxide emissions worldwide. To mitigate the emissions of SO2, scrubbing process employing liquid absorbents is considered as an alternative method in addition to the flue gas desulfurization (FGD). Room temperature ionic liquids (RTILs) have been demonstrated to absorb SO2 effectively. Tunable psychochemical properties derived from the combinations of tailored ionic components and non-volatility of RTILs resulted from the coulombic force stabilization are the key features making these materials more attractive than volatile organics for SO2 capture. Some literatures suggest that the formation of specific interactions such as Lewis acid-base interactions control the SO2 solubility. Thus, the presence of SO2-philic groups on the molecular structure of RTILs is required to achieve high SO2 solubility. In our group, imidazolium-based cations containing various pendant groups with capabilities to form specific yet reversible interactions with SO2 combined with [MeSO3]- as the anion were synthesized. The solubility measurements for SO2 are presented and the effects of the cation structure on the absorption-desorption processes are discussed.

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

Metal-free membranes for the separation of CO2/CH4 mixtures: Imidazolium based-ionic liquids as CO2 transport carriers

이진규, 김진형, 정민석, 김훈식

경희대 화학과

Imidazolium-based ionic liquids with a basic anion were shown to be highly effective carbon dioxide transport carriers for the selective separation of carbon dioxide in methane through membranes. The highest selectivity of 35 was attained when 1-{2-[2-(2-Methylethoxy)ethoxy]ethyl}-3-methylimidazolium methylsulfonate was used as the transport carrier.

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

Ionic liquid catalyzed urea synthesis by the carboxylation of amine

심유나, 김훈식, 정민석

경희대 화학과

Ionic liquid was used in the synthesis of 1,3-disubstituted ureas from the carboxylation of amines by CO2. The types of both cations and anions of IL influenced in the carboxylation reaction of 1,3-dibutylurea. We suggested the importance of the interaction between cation of ionic liquids employed and the carbonyl oxygen of CO2. For the imidazolium series ILs, the yield of DBU increased with increasing basicity of the anion.

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발표코드: **IND.P-6**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

New attempt for Synthesis of Tetraacetylethyleneamin(TAED)

조원제, 서용성, 조보배, 유국현

동국대 화학과

Tetraacetylethyleneamin(이하 TAED)는 찬물세탁시 SPO 또는 SBO 같은 표백제의 산소발생반응시 촉매작용을 일으키는 촉매로 사용된다. TAED 는 1900 년대 초 독일에서 개발되어 전세계 세탁세제분야에 모두 사용될 만큼 그 효용성이 입증되었다. 현재 상업적 TAED 합성을 위해서는 높은 몰수의 Acetic anhydride 를 사용하는 방법이 이용되고 있다. 본 연구는 상업적 합성시 문제가 되는 고농도의 Acetic anhydride 사용을 줄이며 연속생산이 가능한 새로운 합성 시스템에 관한 연구를 시도하고자 한다. 본 연구의 새로운 시도는 일반적인 합성반응(Batch reastion)시 반응계내부 반응물과 생성물의 농도 평형 상태로 인해 발생되는 부 반응물에 관한 문제점을 해결하여 부반응물의 농도가 반응계에 영향을 주지 않도록 하는 합성계를 고안 함으로서 1:2 정반응비의 합성이 가능한 TAED 합성에 관한 연구이다.

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Effect of Metal Oxide Doping on CO_2 Adsorption Behaviors of Activated Carbon Fibers

맹룡월, 박수진

인하대 화학과

In this work, activated carbon fibers (ACFs) were chemical treated with metal oxide. The CO_2 adsorption capacity of high surface area of ACFs-based adsorbents before and after chemical modification at low and high temperature have been studied. The effects of surface chemical treatments on the micropore structures of ACFs were investigated by N_2 /77K full isotherms at 1 atm. The CO_2 adsorption capacity was measured by CO_2 isothermal adsorption at 298 K and 573 K. In the result, the high adsorption capacity adsorbents for CO_2 at high temperature have been developed by introducing metal oxide on ACFs-based adsorbents.

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Preparation and Characterization of Nanoporous Carbons for CO_2 Adsorption

맹룡월, 박수진

인하대 화학과

In this work, nanoporous carbon materials (NCMs) with a high surface area were directly prepared from polymer precursors without any stabilization and activation processes. Carbon precursor was mixed with metal oxide precursor in different ratios, and heat-treated at high temperature in inert atmosphere. The effects of metal oxide contents on the pore structures of NCMs were investigated by N_2/77K full isotherms at 1 atm. The CO_2 adsorption capacity was measured by CO_2 isothermal adsorption at 298 K/1atm. From the results, it was found that the metal oxide contents have a major influence on CO_2 adsorption capacity and textural properties of NCMs.

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Preparation and Electrochemical Performance of Mesoporous Carbon Fibers through Silica Template

정기호, 박수진

인하대 화학과

In this work, the electrochemical performances of mesoporous carbon fibers (MCFs) prepared through templating method were studied. The carbon fibers were fabricated by electrospinning with the mixture of polyacrylonitrile and silica in dimethylformamide, and porous structures of the fibers were obtained by silica etching. The electrochemical properties of the MCFs were evaluated by cyclic voltammetry (CV) measurement. From the results, it was revealed that the specific surface area and pore volume were increased with silica content, resulting from the well-developed mesopores. In addition, it was found that the MCFs prepared with 30 wt.% silica were shown a maximum specific capacitance at low current density. Therefore, it could be concluded that the improved textural properties of MCFs, mainly mesopores, had an effect on the electrochemical performance for electric double layer capacitor.

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Influence of Activation Temperature on Electrochemical Properties of Activated Carbon Nanofibers for Electric Double Layer Capacitor

정기호, 박수진

인하대 화학과

In this work, carbon nanofibers (CNFs) were modified using a metal hydroxide in order to obtain a high surface area. The CNFs were prepared with poly(amideimide) by electrospinning technique. Morphologies and textural properties of the activated carbon nanofibers (ACNFs) were investigated by using scanning electron microscopy (SEM) and a N_2 adsorption analyzer at 77 K. The electrochemical properties of the ACNFs were also confirmed by cyclic voltammetry (CV) measurement. As a result, the activation temperature was a major influence on textural properties of the fibers. Also, the chemical activation of the CNFs led to an increase of capacitance as compared with pristine CNFs. Consequently, it was indicated that the chemical activation was one of the most effective methods to develop the textural properties, as well as to enhance the electrochemical capacities of CNFs.

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Alkali metal promoted Ag-aluminina catalysts for the selective catalytic reduction of NOx using methane: Effect of SO2 gas stream

유창용, *하헌필, *배현숙, **K.Narayana Rao, ***최희락

*부경대 재료공학과 *KIST 기능재료센터 **Indian Institute of Chemical Technology ***부경대 신소재공학부*

SO2 에 대한 내피독특성이 우수한 Ag/Al2O3 촉매를 제조한 후 CH4 를 환원제로 사용하여 촉매활성을 측정하였다. 한편, 촉매의 Selectivity 와 Life time 을 향상 시키고자 IMP(impregnation)법으로 Na, K, Cs 를 첨가하여 촉매를 제조시 이들이 촉매특성에 미치는 영향을 알아보았다. NOx 의 N2 전환률 측정은 400-700℃에서 실시하였고, SO2 의 영향에 대해서 알아보기 위해 SO2 를 흘려가며 촉매의 전환률 특성을 확인해 보았다. 이중 K 를 담지한 Ag/Al2O3 는 SO2 흘려주었을 때, 우수한 특성을 얻을 수 있었다. 촉매의 물리화학적 특성을 분석하기 위해 BET-SA, ICP, XRD, In-situ-IR, TPD 분석을 실시하였다.

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Antimony catalyst supported on V2O5/TiO2 for NH3-SCR at low temperature

이경주, *하헌필, *배현숙, **유창용

*고려대 화공생명공학과 *KIST 기능재료센터 **부경대 재료공학과*

Generally, SCR system shows high NOx removal efficiency at 300~400℃. But SCR system is required for operating at low temperatures. Besides NH3 slip is more increased over the catalysts which have low activities at low temperatures. It can cause NH4HSO4 formation by the reaction with H2O and SO2. SO2 is formed from both the oxidation of sulfur contained in fossil fuels and industrial processes that treat and produce sulfur-containing compounds. If SO2 is present in the combustion gases it can be oxidised to SO3 over the catalyst. This research is to develop the catalyst having improved deNOx activity at low temperatures and high tolerance against SO2 deactivation. As results of SCR experiment, Sb added V2O5/TiO2 catalyst showed the best SCR activity at low temperatures than the activities of other candidates added V2O5/TiO2 catalysts. And as results of SO2 deactivation experiment, Sb added V2O5/TiO2 catalyst showed high tolerance against SO2 deactivation. Sb is suggested as the promoter for low temperature sulfur tolerable deNOx catalyst based on V2O5/TiO2.

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수열방법을 통한 마이크로 구형 수산화마그네슘의 합성

최세범, *박민규, **유현웅

*충북대 공업화학과 *충북대 공업화학 **한국표준과학연구원 전략기술연구부*

수산화마그네슘계 물질은 산화마그네슘을 제조하기 위한 전구체로서 생성조건에 따라 wire, needle, rod, 및 lamella 등에 다양한 형상과 크기 등이 만들어 진다. 이때 생성된 형상은 소성을 통해 산화마그네슘으로 변환 시에도 그대로 유지되며, 각 형상에 따라 촉매, 난연제, 기능성 첨가제, 초전도체 등에 다양한 분야로 사용이 가능하다. 본 연구는 수열방법을 통해 마그네슘 화합물과 암모니아수를 재료로 이온반응 및 침전과정 중에 완충용액의 역할을 살펴보고, 반응조건에 따라 다양한 형태와 크기의 수산화마그네슘 나노 입자를 합성하였다. 이들 물질은 나노 라멜라가 적층하여 다양한 형상과 크기의 마이크로 구형 입자를 형성하며, 이들 입자의 표면 특성 및 결합특성은 주사전자현미경(SEM), 적외선분광기(FT-IR), 공초점라만현미경을 이용하여 확인하였다.

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Asymmetric Anthracene-Based Blue Host Materials: Synthesis and Electroluminescence Properties of 9-(2-naphthyl)-10-arylanthracenes

위경량

고려대 소재화학과

A series of bulky aryl substituted asymmetric anthracene blue host material, 9-(2-naphthyl)-10-(3-(1-naphthyl)phenyl)anthracene, where phenyl was varied from H (5a), Me (5b), Ph (5e), and 1-Naph (5f) at the 6-position and Me (5c) at the 2-position, has been synthesized by suzuki coupling reaction between 10-(2-naphthyl)anthracene-9-boronic acid and 1-(3-iodophenyl)naphthalene derivatives. The photophysical and electrochemical properties in solution showed that the substituent at 10-positions of anthracene unit do not influence on the blue emission of 420 nm and HOMO-LUMO energy level (5.5-2.5 eV). However, a gradual decrease of bathochromic shift in solid state PL was observed from the increasing of the substituent bulkiness, exhibiting 5e (18 nm) ≤ 5f (19 nm) < 5c (25 nm) ≤ 5b (26 nm) < 5a (30 nm) < 5d (41 nm), respectably. When 5a was used as a host material in the multilayered device structure of ITO/DNTPD/NPD/host:dopant (9%)/PyPySPyPy/LiF/Al, enhanced OLED device performance was observed, showing a luminous current efficiency of 9.9 cd/A, power efficiency of 6.3 lm/W at 20 mA/cm2, deep blue color coordinates of (0.14, 0.18), and a 932 h device lifetime at L0=3000 cd/m2

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Broadly Absorbing Sensitizers with Bithiophinosilole as Spacer: Synthesis and Application for High-Efficiency Water Splitting Hydrogen Generation

전지송, 위경량, 한원식, 박종진, 강상욱

고려대 소재화학과

Considerable attention has been paid to semiconductor TiO2 in connection to the creation of clean energy, typically hydrogen evolution from water and electricity generation by solar cells under solar-light illumination. Due to little visible-light absorption by TiO2, dye modification has been used to make TiO2 active to visible-light excitation, typically in dye-sensitized H2 generation using platinized TiO2 particles (Pt/TiO2).Two new organic sensitizers STPH and SMOM with bithiophinosilole as spacer were synthesized. Their absorption spectra were broad with long wavelength absorption 370–657 nm, due to the planarity of bithiophinosilole spacer group, and HOMO level of 0.6–0.8 eV. The hydrogen generation efficiencies of the dyes grafted to Pt/TiO2 were measured, comparable to 3-(5'-{4-[Bis-(4-methoxymethyl-phenyl)-amino]-phenyl}-[2,2']bithiophenyl-5-yl)-2-cyanoacrylic acid (DMOM), fabricated and measured under the same experimental conditions. We found that the efficiency of hydrogen generation was of the order SMOM > STPH. The maximum hydrogen generation was about 368 μL with SMOM.

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Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Visible-Light Hydrogen Generation Based on Pt/TiO_2 particle

김주은, 위경량, 강상욱

고려대 소재화학과

Due to little visible-light absorption by TiO_2, dye modification has been used to make TiO_2 active to visible-light excitation, typically in dye-sensitized H_2 generation using platinized TiO_2 particles (Pt/TiO_2). Recently, we reported the synthesis and characterization of a hydrophilic organic dye (JED2) that gave total hydrogen evolution of 80 *u*mol. In this report, to extend the spectral response of chromophore toward the red region and to fine-tune the HOMO and the LUMO energy levels of the sensitizer a series of dyes was designed. And, all organic dyes, featuring oligothiophene (mono-, JED1; bis-, JED2; tri-, JED3; tetra-, JED4) linker and methoxymethyl substituted arylamines donor at the 4-position, have been successfully synthesized. These compounds were fully characterized by photophysical, electrochemical, and theoretical computational methods. As a result of this modification, a characteristic difference was observed not only on the molecule spectroscopic and electrochemical properties but also on the hydrogen-generation efficiencies.

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TiO_2-mediated Photocatalytic Water-splitting Using Benzothiadiazole-based Organic Dye for Hydrogen Production

황아름, 김현영, *한원식, *박종진, *강상욱

*고려대 신소재화학과 *고려대 소재화학과*

To improve the light-harvesting efficiency and water miscibility in sensitized H_2 generation based on Pt/TiO_2 catalysts, a series benzothiadiazole-based organic dye has been designed and synthesized. Among the series, hydrophilic group was attached to prevent conformation/aggregation behavior of the dye adsorbed on the TiO_2 surface, which have critical effects on the electron-transfer and chemical processes involved in H_2 generation. In this study, detailed investigation on the relationship between the dye structure and performance of hydrogen generation is described. As a result, synthesized dye absorbed in the near 650 nm, and hydrophilic character lead higher sensitization activity in hydrogen generation. In addition, the stability of $OD/Pt/TiO_2$ catalysts was robust over the extended catalytic cycles and this property was confirmed by DRS spectroscopy.

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A Novel Organic Dye Incorporating a Low-band-gap Chromophore Based on Hydrophlic-Functionalized Triphenylamine for Efficient Hydrogen Generation

한중규, *김성관, *한원식, 김현영, *박종진, *강상욱

*고려대 신소재화학과 *고려대 소재화학과*

This study aims to explore the significance of hydrophilic and steric characteristics of organic dyes in sensitized H2 generation based on Pt/TiO2 catalysts using a series of (E)-2-cyano-3-(7-(5'-(4-(p,p'-bis(R-phenyl)amino)phenyl)-2,2'-bithiophen-5-yl)benzo[c][1,2,5]thiadiazol-4-yl)acrylic acid dyes, where R = H (HKD1) and CH2OCH3 (HKD2). Synthesized organic dyes were applied to TiO2-mediated hydrogen generation under visible light irradiation. The introduction of benzothiadiazole, as a spacer, showed the maximum UV/Vis absorption of HKD1 and HKD2 at 511 nm and 515 nm, respectively. In this study, detailed investigation on the relationship between the dye structure and performance of hydrogen generation is described. The hydrogen generation efficiencies and optimum amounts of the dyes grafted to Pt/TiO2 were affected substantially by the hydrophilicity of dye; hydrophilic HKD2 showed higher sensitization activity at a lower loading than hydrophobic HKD1.

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Development of chemical hydrogen materials for hydrogen fuel cell applications: Palladium Catalysts for Dehydrogenation of Ammonia Borane with Preferential B-H Activation

김태영, 강상욱, 김성관, 김태진, 한원식

고려대 소재화학과

Ammonia borane (NH3BH3) has emerged as a potential candidate to meet the requirements of onboard chemical hydrogen storage (CHS) systems. However, the challenge of finding a suitable method for releasing sufficient amount of hydrogen at the required rates persists. This study focused on the development of high performance catalysts for the dehydrogenation of AB. Cationic Pd(II) complexes were the most efficient catalysts, releasing 2.0 equiv H2 at room temperature within 60 s. The catalysts comprised Pd(II) and a charge-balancing weakly-coordinating counter anion, BF4-. Catalyst activities were fine-tuned with allyl, 2,4-hexadiene, and acetonitrile ancillary ligands. The H2 purity and quantity were determined using quadrupole mass spectroscopy (QMS) and a mass flow meter (MFM), respectively. Kinetic isotope effect (KIE) values of 2.5, 8.2, and 9.5 were measured for ND3BH3, NH3BD3, and ND3BD3, respectively, indicating that the B-H and B-D bonds weakened considerably. To further consolidate the facile B-H activation, a series of alkyl ABs was examined in order to show that the H2 release amount was dependent on the number of hydrogen atoms at the boron atom. A proposal for the first dehydrogenation mechanism by DFT calculations and detailed descriptions of the solid state 11B spectra of the AB and alkylated AB spent fuels are now presented in this study.

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Development of Single-Site Catalyst for EPDM Polymerization: Synthesis and Structural Characterization of New Types of High Performance Half-Metallocene Catalysts

임방현, 김태진, 김성관, 한원식, 강상욱

고려대 소재화학과

Ligand effects on the catalytic activity [and propylene and nobornadiene incorporation] for both ethylene polymerization and ethylene/propylene/norbornadiene (EPDM) ter-polymerization using half-titanocenes (titanium half-sandwich complexes) containing 2-alkyl phenoxy ligand of type Cp'TiCl2(2-R-PhO) catalyst systems have been investigated. Cp*TiCl2(2-R-PhO) (R= Me Cp*Me, iPr Cp*Pr, tBu Cp*Bu, Ph Cp*Ph) were prepared and identified; the structures of Cp*Pr and Cp*Ph were determined by X-ray crystallography. The metal coordination geometry of each compound is best described as pseudo-tetrahedral, with the Cp* ring and 2-R-PhO and chloride ligands occupying three leg positions in a piano-stool geometry. The Ti–O bond length of Cp*Ph [1.784(2) Å] was similar to those found in the complex CpPh [1.782(1) Å]. The catalytic activity for ethylene homo-polymerization increased in the order: Cp*Ph [6.6 Kg/(mmol of Ti•h), in toluene, ethylene 4 atm, 80 °C, 30 sec] > Cp*Pr [5.1 Kg/(mmol of Ti•h)] > Cp*Me [5.0 Kg/(mmol of Ti•h)] > Cp*Bu [2.2 Kg/(mmol of Ti•h)]. The effect of the cyclopentadienyl fragment and ortho substituent phenoxy ligands in the ter-polymerization of EPDM by CpMe–Cp*Ph catalyst systems has been explored. The phenoxy system showed the high catalytic activity for EPDM terpolymerization, affording a high molecular weight with a unimodal molecular weight distribution and higher propylene incorporation.

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High molar extinction coefficient organic sensitizers for visible-light hydrogen generation based on platinized TiO2 particles

김애리, 위경량, 한원식, 박종진, 강상욱

고려대 소재화학과

Utilization of solar energy to produce hydrogen gas from water has long been considered the ultimate solution. Since the discovery in 1971 that TiO2 could act as a photochemical water-splitting catalyst, over 100 photocatalysts have been reported. However, for practical applications, pure TiO2 is not a good candidate, because it is only active under ultraviolet (UV) irradiation in order to overcome the band gap of 3.2 eV for anatase phase. Therefore, dye sensitized platinized TiO2 nanocrystalline, where dye has hydrophilic characters, is required if we want to use TiO2 as a water-splitting catalyst under visible light irradiation. In this study, a series of thipohene-vinyl-thipohene linker substituted organic dye, (E)-2-cyano-3-(5-((E)-2-(5-(4-(diphenylamino)phenyl)thiophen-2-yl)vinyl)thiophen-2-yl)acrylic acid, where diphenylamino was varied from -H (ALD1) and -CH2OCH3 (ALD2) at the 4-position of phenyl, was successfully prepared. The maximum UV/Vis absorption of ALD1 and ALD2 showed 472 and 477 nm, respectively, with high molar extinction coefficient (′ , M-1cm-1= 81,000). The hydrogen-generation efficiencies and optimum amounts of the dyes grafted to Pt/TiO2 were affected substantially by the hydrophilic and steric effects; moderately hydrophilic ALD2 showed higher sensitization activity.

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The Relationship between the Functional Group of Organic Dye and the Performance of Hydrogen Generation under Visible-light Irradiation

김현영

고려대 신소재화학과

To explore the hydrophilic and fluorophilic characteristics of organic dyes in sensitized H2 generation based on Pt/TiO2 catalysts, we synthesized (*E*)-3-(5'-(4-(*p*,*p*'-R)phenyl)amino)phenyl)-2,2'-bithiophen-5-yl)-2-cyanoacrylic acid dyes, where R = CH_2OCH_3 (DMOM) and $CH_2OCH_2CF_3$ (TFOM). Both of catalysts were systematically tested their visible light reactivity for hydrogen production in aqueous suspension (with EDTA as an electron donor) under $\lambda > 420$ nm illumination. The relationship between the dye structure and performance of hydrogen generation is described in detail. In particular, the formation of organic dyes on TiO_2 surface was investigated by using polarized UV/Vis spectroscopic. The result showed that fluorophilic character led the decrement of the sensitization activity. Furthermore, (*E*)-3-(5'-(4-(bis(4-(methoxymethyl)phenyl)amino)phenyl)-4,4'-bis(methoxymethyl)-2,2'-bithiophen-5-yl)-2-cyanoacrylic acid (TMOM) was prepared to maximize the hydrophilic effect and showed highest performance of hydrogen generation.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND.P-23**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Activity Control by Electronic Alteration at 2-Phenyl Group and 4-Position of the Phenoxy Ligand in Half-Metallocene Titanium(IV) Complexes

김태진, 김성관, 한원식, 임방현, 강상욱

고려대 소재화학과

Electronic alteration was focused at the three different sites on 2-phenyl phenoxy ligand, one at the 2-position phenyl group (Type II) and the other two at the 4-position with a direct substitution (Type I) or substitution through another phenyl ring (Type III). This resulted in a wide variety of electronically tuned titanium complexes comprised of 2-Ph-4-X-PhO (Type I, X = F, 5a; Cl, 5b; Me, 5c; iPr, 5d; tBu, 5e; OMe, 5f), 2-(4'-X-Ph)-PhO (Type II, X = CF3, 10a; F, 10c; OMe, 10d) and 2-(2',4'-F2-Ph)-PhO 10b, and bridging phenyl substituents, 2-Ph-4-(2',4'-F2-Ph)PhO 13a and 2-Ph-4-(4'-X-Ph)PhO (Type III, X = F, 13b; Cl, 13c; H, 13d; tBu, 13e; NMe2, 13f). In Type I, a systematic electronic perturbation was confirmed by Hammet plot of the para substituents (σp) with respect to the reduction potential at the titanium metal. As catalysts for ethylene homo-polymerization at high temperature (140 ´ C), para- and ortho-substituted Type I and Type II showed higher activities than that of Type III. Further, in general 2-phenylphenoxy system with electron-withdrawing groups showed superior activities to with electron-withdrawing groups and in each system fluorine substitution gave rise to the best activity with 37.2, 34.2, and 20.4 Kg/(mmol of Ti•h) for 5a, 10a, and 13a, respectively. As the substituent becomes more electrons withdrawing, higher molecular weight was obtained: In the case of 5a, Mw= 372,000 exceeded over to the value of Mw= 222,000 for 5f. In particular, 5a exhibited the ethylene copolymerization catalytic activity of 39.0 Kg/(mmol of Ti•h) with 1-octene, surpassing the reference catalyst Cp*Ti(2-Ph-PhO)Cl2 of 34.2 Kg/(mmol of Ti•h).

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

세척력이 우수하고 증류, 재생이 가능한 지속적인 난연성 탄화수소 세정제의 개발.

유영

국민대 화학과

기존의 사용중인 세척 세정제의 단점을 보안하기 위해 염화물 세정제가 아닌, 탄화수소 세정제를 개발 하게 되었다. 기존의 세제의 세정력보다 우수한 세정력을 가지고, 또한 화재에 대한 위험성을 낮춘 난연성세제의 개발에 중점을 두었음. 세척 폐액의 처리가 간편할 뿐아니라 세제의 증발이 적어 소모량이 적고 진공상태의 증류, 재생이 가능하여 경제적으로 우수하다.

한국화학회 KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND.P-25**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

고부가 청정자원으로 활용 가능한 MFB 정제

이윤아

국민대 화학과

p-xylene 산화과정을 통해 dimethylterephthalate(DMT) 생성시 부산물로 나오는 methylformylbenzoate(MFB)를 정제하기 위한 방법으로, Hydroxylamine salt 와 MFB mixture 를 합성시켜 순수한 MHB 를 얻어낸다.그 뒤, MHB 를 MFB 로 환원시킴으로써, 고순도의 methylformylbenzoate 를 얻어낸다.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND.P-26**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Development of chemical hydrogen materials for hydrogen fuel cell applications: Palladium Catalysts for Dehydrogenation of Ammonia Triborane in nonaqueous medium

김성관, 김태영, 김태진, 한원식, 강상욱

고려대 소재화학과

The high hydrogen release capacity that could potentially be achieved by ammonia triborane ($NH_3B_3H_7$, ATB) oxidative-hydrolysis, eq 1, (9.7 materials wt % H_2) or thermolysis, eq 2, (17.7 materials wt % H_2) also makes it an attractive candidate for chemical hydrogen storage. During the hydrolysis and dehydrogenation processes, B–H bonds are cleaved and the resulting products are composed of mainly B–O. This pathway may make the regeneration of spent fuel economically and energetically inefficient. Cationic Pd(II) complexes catalyzed the dehydrogenation of ammonia borane in the most efficient manner with the release of 2.0 equiv H_2 in less than 60 s at 25 °C. Most hydrogens were obtained from the boron atom of the ammonia-borane. Recent work in our group into cationic palladium catalysts with preferential B-H activation has led to our initial studies of ATB dehydrogenation properties in non aqueous medium. The introduction of a catalytic amount of Pd catalyst onto a solution of ATB in tetraglyme produced a rapid effervescence of H_2 gas from the solution. The H_2 purity and quantity were determined using quadrupole mass spectroscopy (QMS) and a mass flow meter (MFM), respectively. The progress of this reaction was monitored using ^{11}B NMR.

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장소: 대구엑스코
발표코드: **IND.P-27**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A method for preparing selectivity enhanced silicotitanate

전종원

안동대 응용화학과

Silicotitanate have been known as adsorbent for cations from nuclear wastewater. Silicotitanate can be a effective alternatives for removal of inorganic radionuclide through enhanced sorption capacity and selectivity. Synthesis of the adsorbent with high sorption capacity and high selectivity required several accurate conditions and materials such as temperature, ratio of materials, and pressure. We have studied post-treatment method in order to enhance the capacity and selectivity of silicotitanate which is prepared simple synthetic method. H-silicotitanate showed enhanced selectivity for some cations.

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장소: 대구엑스코
발표코드: **IND.P-28**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication of higher-order clusters, supraparticles, and supraballs by self-organization of colloidal nanospheres inside emulsion droplet

조영상, *이기라

*한국기계연구원 부설 재료연구소 기능재료연구본부 나노기능분말그룹 *충북대 공업화학과*

Monodisperse cross-linked polystyrene nanospheres were self-organized to fabricate colloidal aggregates from toluene-in-water emulsion droplets as confined geometry, as shown in the schematic diagram of Fig. 1. During the evaporation of toluene by heating, the polystyrene nanospheres were packed into higher-order clusters, supraparticles with intermediate packing ordering or supraballs with hexagonally ordered structures, depending on the size of emulsion droplets or the number of constituent particles inside droplets, as examplified in the SEM images of Fig. 2. The structure of the higher-order clusters was also predicted using Surface Evolver simulation tool, as shown in Fig. 3.

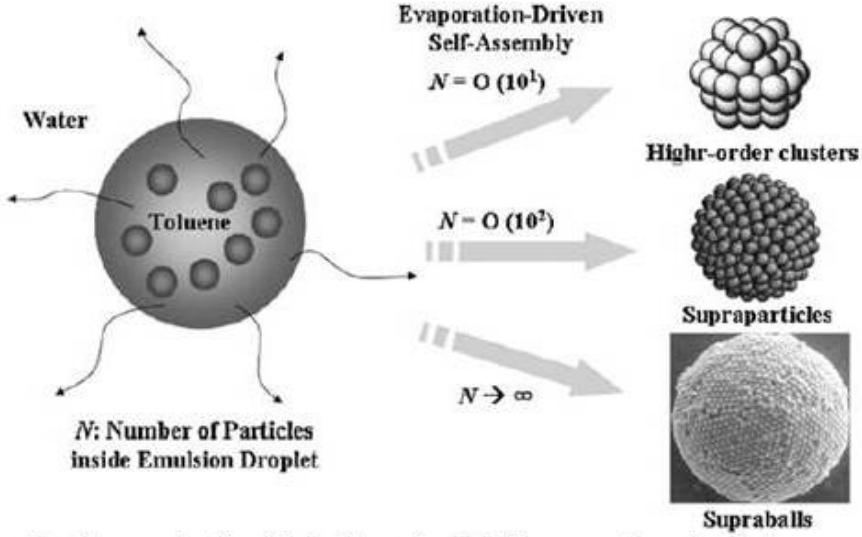


Fig. 1. Schematic diagram for the fabrication of colloidal aggregates of polystyrene nanospheres from toluene-in-water emulsions by evaporation-induced self-assembly

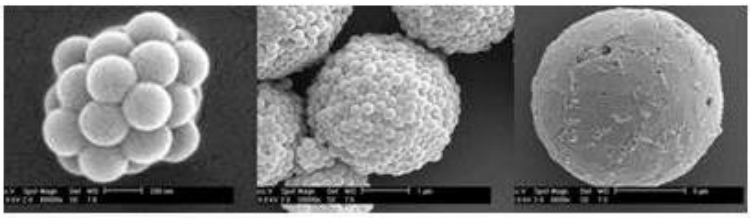


Fig. 2. Scanning electron micrographs of higher-order clusters, supraparticles, and supraballs made of polystyrene nanospheres

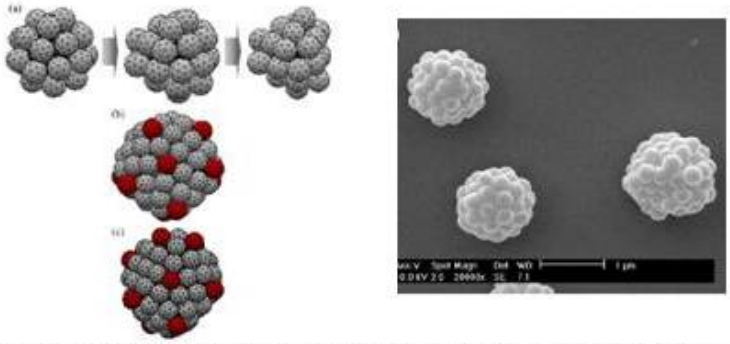


Fig. 3. Surface Evolver simulation of the self-assembled structures with constituent number of particles, N = 24 (a), 60 (b), and 72 (c). (d) Scanning electron micrograph of supraparticles

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND.P-29**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A method for preparing selectivity enhanced silicotitanate

전종원, *김영훈, *권순덕, *조대호, *임기영

*안동대 응용화학과 *안동대 환경공학과*

Silicotitanate have been known as adsorbent for cations from nuclear wastewater. Silicotitanate can be a effective alternatives for removal of inorganic radionuclide through enhanced sorption capacity and selectivity. Synthesis of the adsorbent with high sorption capacity and high selectivity required several accurate conditions and materials such as temperature, ratio of materials, and pressure. We have studied post-treatment method in order to enhance the capacity and selectivity of silicotitanate which is prepared simple synthetic method. H-silicotitanate showed enhanced selectivity for some cations.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **IND.P-30**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A Novel Cationic Surfactant Having Two Quaternary Ammonium Ions

강은경, *박종목, *강호철, *이병민

*과학기술연합대학원대 청정화학및 생물학전공 *한국화학연구원 그린화학연구단*

Generally cationic surfactants are well adsorbed on the fabric surface because synthetic fiber surface is negatively charged in the water usually. So, cationic surfactants have been widely used as fabric softener, anti-static agent and detergent. In this study, a novel cationic surfactant was synthesized and its surface-active properties were evaluated. N,N-bis(3-n-dodecyloxy-2-hydroxypropyl)-N,N-dimethyl-1,3-propylenediamine(BDPD) was prepared quantitatively by the condensation reaction between n-dodecylglycidyl ether and 3-(dimethylamino)-1-propylamine under mild conditions without a solvent. The BDPD was quaternized with dimethyl sulfate. The structure of BDPD was characterized by H NMR, FAB mass and FT-IR.

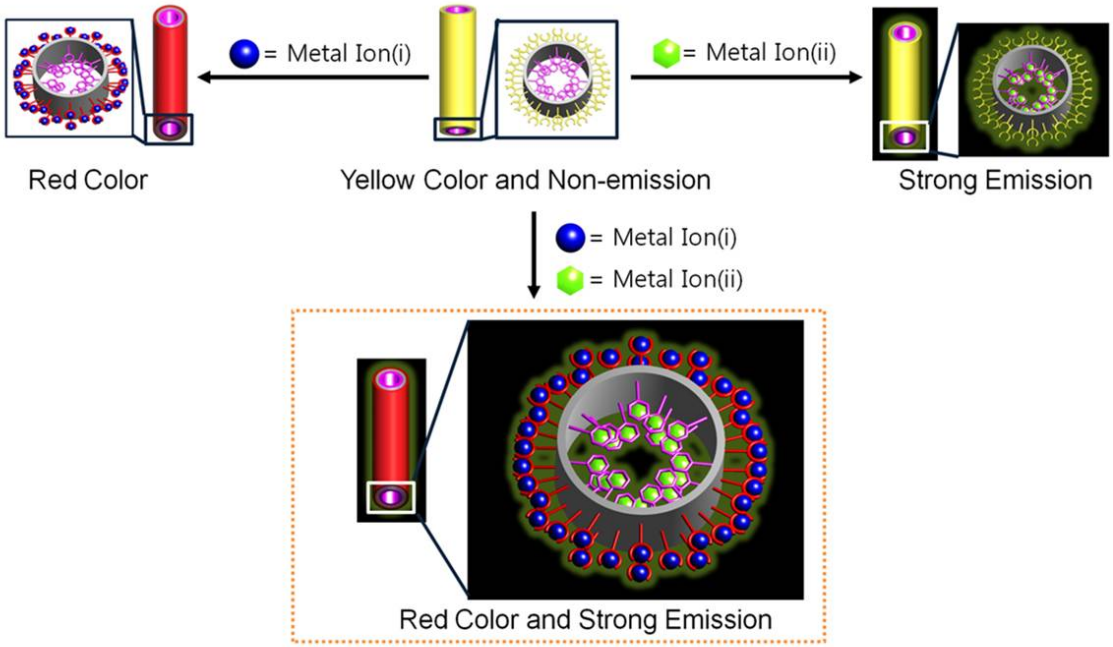
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-1**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of Silica Nanotue Immobilized Two Different-type Ligands as a Selective Chmosensor

서성민, 정종화

경상대 화학과

We synthesized two different chromogenic ligands, which have selectively recognized for Pb^{2+} and Hg^{2+} ions, respectively. Two different-type lignads were attached onto the inner and outer surface of silica nanotubes by sol-gel grafting reaction. Two different-type ligands immobilized silica nanotubes(T-SNTs) were characterized by SEM, TEM, TOF-SIMS, and FT-IR. We observed the chromogenic and fluorogenic changed of T-SNTs upon the addition of metal ions in aqueous solution. T-SNTs selectively recognized for Pb^{2+} and Hg^{2+} ions by each ligands attached onto surface of silica nanotubes.



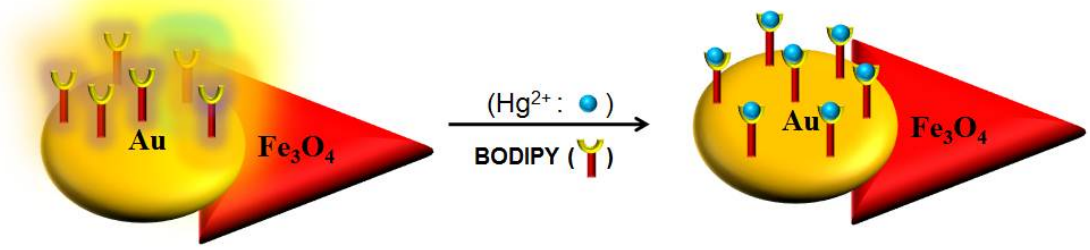
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-2**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

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

손현종, 정종화

경상대 화학과

Heavy metal ion pollution poses severe risks for human healt hand the environment. Mercury contamination is widespread and occurs through a variety of natural and anthropogenic sources including oceanic and volcanic emission, gold mining, solid waste incineration, and the combustion of fossil fuels. Once introduced into the marine environment, bacteria convert inorganic mercury into methylmercury, which enters the food chain and accumulates in higher organisms, especially in large edible fish. Methylmercury is neurotoxic and has been implicated as a cause of prenatal brain damage, various cognitive and motion disorders and Minamata disease. Our increased understanding of the deleterious effects of mercury exposure has sparked interest in the development of new tools for detecting Hg(II) in the environment.The BODIPY derivative was synthesized of the benzoylchloride, 2,4-dimethylpyrrole, BF_3-OEt_2, 5-(1,2-dithiolan-3-yl)pentane-1-thiol. we prepred binary metal nanoparticles(Au/ Fe_3O_4) as a spporting metarial. Then, The BODIPY was immobilized onto gold and Fe_3O_4nanoparticles by sol-gel reaction. The ability of 1 to sense metal ion was studied by addition of various metal ions in results the change of color was in mecury



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일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-3**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Prepartation of benzo-18-crown-6 immoblized mesoporous silica as nanocarrier

최영란, 박경원, 서무룡, 정종화

경상대 화학과

Inorganic nanomaterials have found broad applications in biological and environmental fields such as biolabeling, imaging, drug delivery, separation processes, and optical sensing. Benzo 18-crown-6 was immobilized onto the surface of SBA-15 by sol-gel grafting reaction in toluene. The hybrid nanomaterial was characterized by SEM, TEM, FT-IR and solid ^{13}C-NMR. 20 wt% of Benzo 18-crown-6 was attached by measurement of TGA. B18C6-SBA-15 formed complex with alkyl diammonium ion by the hydrogen-bonds. In this symposium, we will explain on preparation of B18C6-SBA-15 in detail.

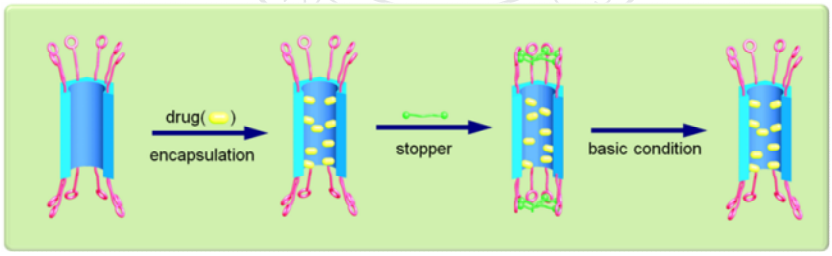


Figure 1. Preparation of B18C16-SBA-15 : (a)SBA-15(B18C6-SBA-15), (b)encapsulation of drug, (c)locking and(d) unlocking.

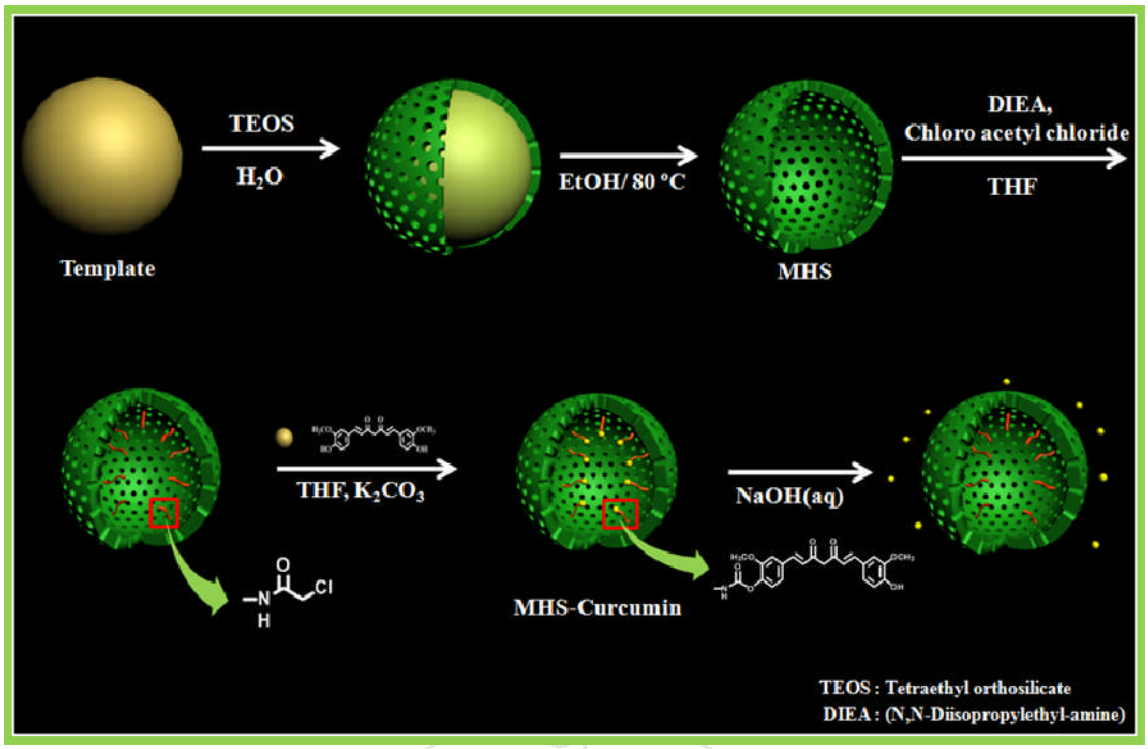
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-4**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of Mesoporous-Type Hollow Silica Spheres by using Template and its Drug Delivery Application

진달샘, 박경원, 서무룡, 정종화

경상대 화학과

The mesoporous hollow silica sphere (MHS) was prepared by using alanine-based amphiphile possessing either a saturated long alkyl chain group or unsaturated groups as a template. MHS was characterized by PXRD, TEM, SEM and BET isotherm analysis. MHS showed mesopore with 4.5 nm and hollow cavity. The curcumin was selectively immobilized onto inner surface of MHS by covalent bond. The curcumin attached onto the inner surface of MHS was released by change of pH into aqueous phase. We will detail discuss onto a fabrication of MHS and its application as drug delivery system in this symposium.



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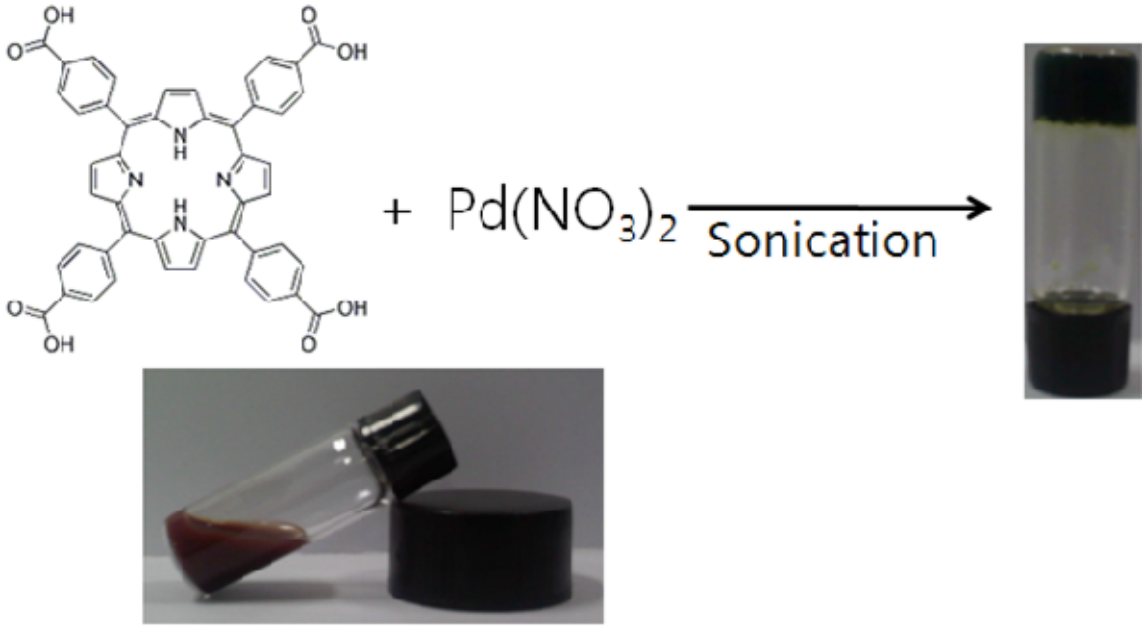
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-5**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of Self-Assembled Metallogel with Palladium Ion as a Catalyst

조영제, *Jagadese J. Vittal, 정종화

*경상대 화학과 *National University of Singapore Singapore and Gyeongsang National University Korea*

Tetrakis(4-carboxyphenyl)porphyrin(TCPP) formed gel in the presence of Pd^{2+} ion without heating process. TCPP-Pd metallo gel was characterized by TEM, FT-IR, UV-Vis spectroscope and Fluorophotometry. The freeze-dried gel exhibits a fibrillar network structure. UV/vis absorption studies illustrate that the TCPP-Pd gel displays a typical π - π^* transition. The fluorescence intensity of the gel in the presence of Pd^{2+} is quenched dramatically with gel formation. Also, this gel acted as a novel and efficient catalyst for Sonogashira reaction. The metallogel may find utility as a novel soft material in biomedical and photochemistry fields.



대한화학회
THE KOREAN CHEMICAL SOCIETY

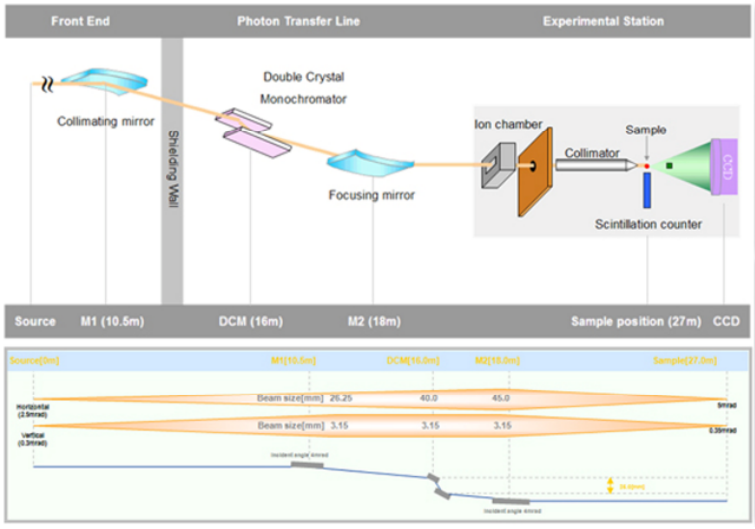
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-6**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Status of 6B Beamline for the Small Molecule X-ray Crystallography at Pohang Accelerator Laboratory

문도현

포항가속기연구소 빔라인부

The 6B beamline at Pohang Accelerator Laboratory in Korea has been designed to operate in the photon-energy range of 6 ~ 17.5 keV (2.0 ~ 0.71Å) based on a bending magnet source. The purpose of this beamline is for X-ray crystallography of small molecule and supramolecule user groups. Operation of this beamline was started from year 2001 as a first synchrotron macromolecule crystallography in Korea and changed to support of small molecule users at year 2009. The synchrotron radiation is powerful light flux its about 10,000 times stronger than commercial lab source(Cu, Mo tube) as well as easily changeable energy range. Through these advantages produced lots of benefit for the chance with collection data of the impossible crystal in the lab. For example, diverse experiments are possible to all kinds of organic/inorganic single crystals, very hollow structure such as MOF or cage structure, very tiny size crystal (~0.01 mm^3), and with large quantity of structural solvents. Also we have installed various convenience stuffs and equipments such as temperature controlled devices (90 ~ 400K; LN2, 9 ~ 120K; LHe), high resolution microscope with DSLR photo system, high sensitivity of large area detector, and high performance data processing server. The status, equipments and several techniques of 6B beamline will be presented on this poster.



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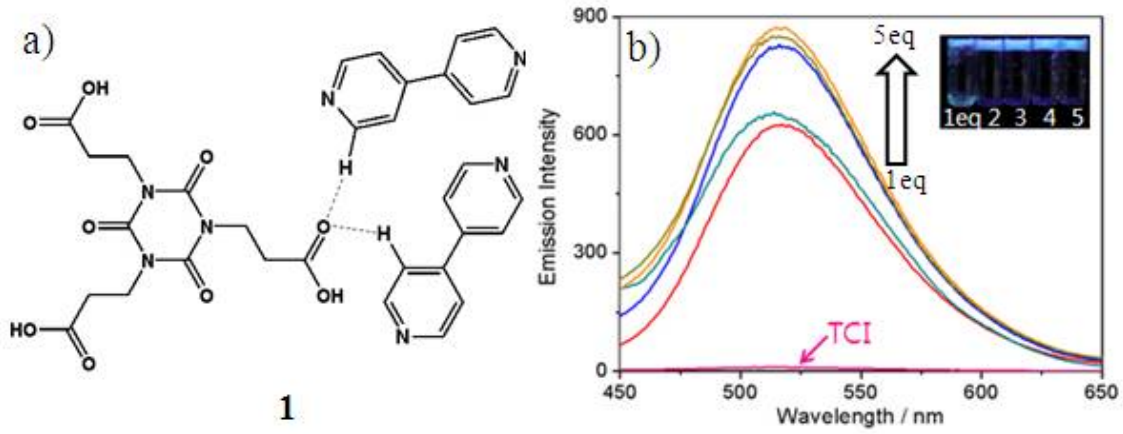
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-7**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Fluorescent enhancement of Tri(2-carboxyethyl)isocyanurate derivative coordination polymeric gel via hydrogen bonding with bipyridine

이혜진, 정종화

경상대 화학과

A solvothermal reaction of 4,4'-bipyridine(bpy) and Tri(2-carboxyethyl)isocyanurate(H_3TCI) forms coordination polymeric gel in MeOH, H_2O. Gel showed fibrous structures and luminescence properties. We monitored fluorescence lifetime by time-resolved fluorescence confocal microscopy. The fluorescence decay of coordination polymeric gel was fit with a single exponential component yielding a lifetime of 3.2 ns, indicating that this emission is fluorescence. These solvothermal reactions by H_3TCI and bpy not only induced gelation, but also led to fluorescence enhancement. Aside from the hydrogen bonding coordination polymeric gel of H_3TCI with bpy, an important intermolecular interaction within these gels is likely to be H-bonding interactions. The crystal structure of 1 consists of one molecule of H_3TCI and one and half molecules of bpy in asymmetric unit. Details of gelation behavior, fluorescence property and X-ray structure will be discussed in the poster presentation.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-8**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Pyridine-based Coordination Polymeric Gel and Its Application for Chloride Anion Sensing

이지하, 서무룡, 정종화

경상대 화학과

we synthesized the pyridine -appended benzene ligand (1). Compound (1) forms gel upon addition of Co^{2+} ion in 0.1M NaOH when mixed two solutions. UV/Vis absorption band of Co^{2+} coordination polymeric gel appears at 480 nm, which is a typical π-π* absorption band. On the other hand, the π-π* absorption band of sol shows a large blue shift in energy to λ=250 nm. Also, the red color of polymeric gel 1 was changed into blue color in the presence of Cl_2gas. Interestingly, the color change of CoBr2 coordination polymer gel upon the addition of chlorine gases such as HCl, $SOCl_2$2, $(CO)_2Cl_2$, and $COCl_2$ (phosgene) was observed from the red to blue in gas phase. Furthermore, sensing of chlorine gases by $CoBr_2$ coordination polymeric gel as chemosensor was studied in gas phase by using UV/Vis spectroscopic technique. The UV/Vis spectrum of $CoBr_2$ coordination polymer gel exhibits absorption band at 303nm with red color, which color indicates the formation of octahedral complexes. Upon addition of small amounts of chlorine is red shifted by 387 nm, a new strong band at 690 nm with blue color, because probably the bromide anions were replaced by chlorine.

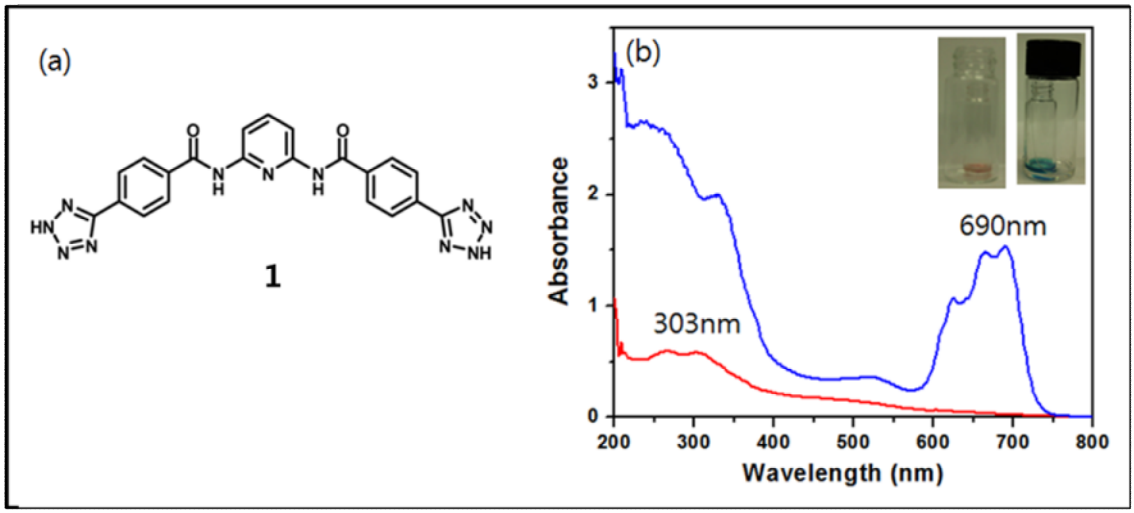


Fig. 1. a) Compound 1, b) UV/Vis spectra of cobalt coordination polymeric gels

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Characterization of coordination polymer gel based on trans-di(4,5-diazafluorene-9-ylimino)dibenzo-18-crown-6 with Zn^{2+} ion

김지향, 서무룡, 정종화

경상대 화학과

Gel are of great importance due to the fact that they are potential materials in numerous application such as drug delivery system (DDS), treatment of waste materials and pollutant, recovery of precious bioactive compounds, catalyst screening, chemical sensing, actuators and tissue engineering. Therefore, we synthesized compound 1 as ligand and its gelation ability was evaluated in the presence of transition metal ions such as Zn^{2+}, Cu^{2+}, Cd^{2+}, Pb^{2+} and Mn^{2+} in organic solvents and H_2O. Compound 1 formed gel in the presence of Zn^{2+} with H_2O/DMSO. In addition, coordination polymer gel 1 was formed with 3, 4 equivalent of Zn^{2+} ion. The coordination polymeric gel 1 induced Zn^{2+} was assessed by various anions such as NO_3^-, ClO_4^-, CH_3COO^-, I^-, and Cl^-. 1 formed coordination polymeric gel with various anions such as NO_3^-, ClO_4^-, CH_3COO^- and I^-. In addition, the morphology of coordination polymer gel 1 was confirmed by SEM and TEM. UV/vis absorption band of Zn^{2+} coordination polymeric gel 1 appears at 482 nm, which is a typical π - π^* absorption band. On the other hand, the π - π^* absorption band of 1 shows 38 nm blue shift. In this symposium, we will discuss on the preparation of coordination polymer gel with transition metal ions and its physical properties.

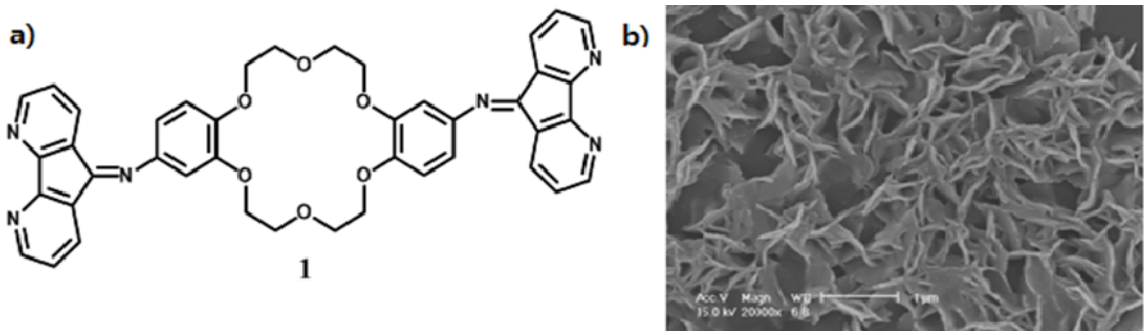

Figure 1. a) Chemical structure of compound 1. b) SEM image of Zn^{2+} Coordination polymeric gel.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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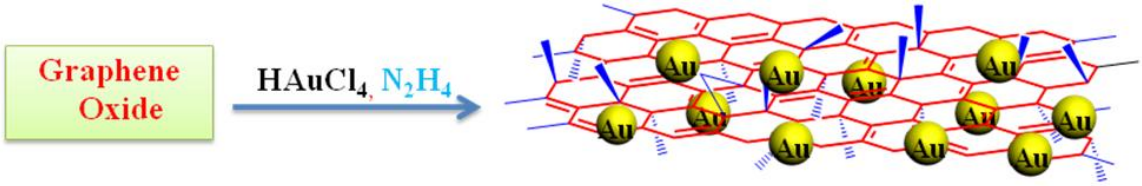
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of Reduced Graphene Oxide and Au nanoparticles

문승진, 박경원, 정종화

경상대 화학과

We prepared the graphene oxide by Hummer's method by it's war characterized by XPS, XRD, and AFM. The graphene oxide showed 1.0nm of thickness by AFM observation. The surface of graphene oxide contained ketone, ester, hydroxy, formyl, and carboxyl groups. In addition Au nanoparticles were deposited on to the surface of graphene oxide.



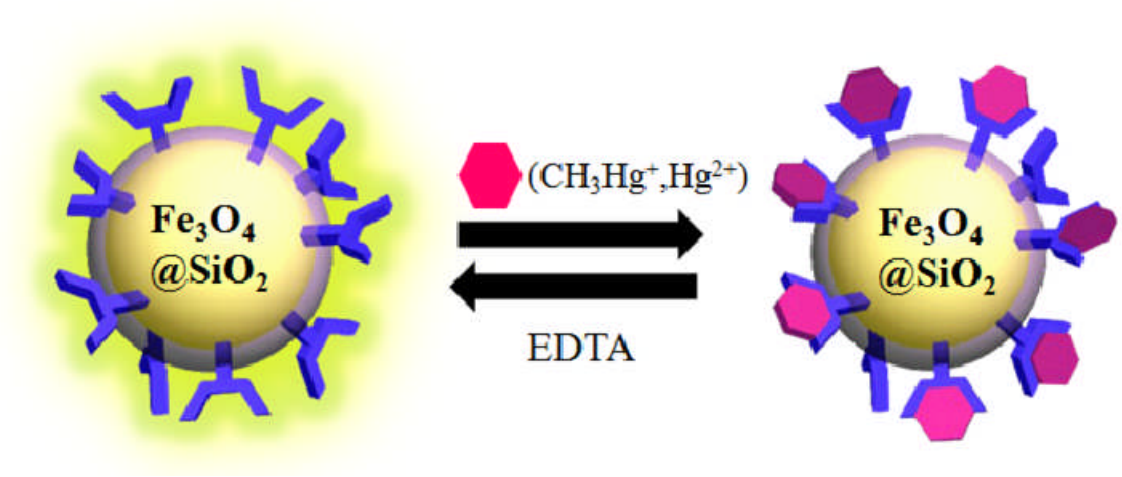
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-11**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Silica-Based Magnetic Nanoparticles for Detection of mercuric ion and methylmercuric ion

박민성, 서성민, *이인수, 정종화

*경상대 화학과 *경희대 응용화학과*

New fluorogenic based aminonaphthalimide-functionalized Fe_3O_4@SiO_2 core/shell magnetic nanoparticles 1 has been prepared, and its abilities to sense and separate metal ions were evaluated by fluorophotometry. The absorption spectrum of free 1 showed a single visible absorption band at 350 nm and a corresponding fluorescence emission maximum at 520 nm. Upon the addition of increasing Hg^{2+} concentrations, 1 showed a large quenching effect with a PET (photoinduced electron transfer,′ < 0.0001) effect in the emission spectra. To determine the amount of Hg^{2+} and CH_3Hg^+ separated by the magnetic silica nanoparticles 1, the amount of Hg^{2+} and CH_3Hg^+ left in the drinking water eluate was determined by ICP-MS. Interestingly, no residual levels of Hg^{2+}′ and CH_3Hg^+ were detectable in drinking water by ICP-MS, suggesting that the designed magnetic silica nanoparticle 1 removed almost 100% of Hg2+ and CH3Hg+. Thus, Fe_3O_4@SiO_2 core/shell nanoparticles 1 can be a potentially useful and effective agent for the selective separation and rapid removal of Hg^{2+} and CH_3Hg^+ from drinking water.



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일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-12**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Various Mono-*N*-functionalized Tetraaza Macrocyclic Copper(II) and Nickel(II) Complexes

강신걸, 김현자

대구대 화학과

The macropolycycle 17-cyanomethyl-3,14-dimethyl-2,6,13,17-tetraazatetracyclo[16.4.1$^{2.6}$.0$^{1.18}$.0$^{7.12}$]tricosane (B) has been prepared by the reaction of 3,14-dimethyl-2,6,13,17-tetraazatetracyclo[16.4.1$^{2.6}$.0$^{1.18}$.0$^{7.12}$]tricosane (A) with 2-bromoacetonitrile. The nickel(II) and copper(II) complexes of 2-cyanomethyl-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (C) bearing one *N*-cyanomethyl pendant arm have been prepared by the reaction of B with the metal ions. The complexes $[Ni(C)]^{2+}$ and $[Cu(C)]^{2+}$ can be used for the preparation various types of mono-*N*-functionalized macrocyclic complexes. Synthesis, characterization, and chemical properties of the mono-*N*-functionalized macrocyclic compounds are presented.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Chemical Properties of Tetraaza Macrocyclic Nickel(II) and Copper(II) Complexes Bearing Ketone Groups

강신걸, 김현자, *곽지훈

*대구대 화학과 *순천대 화학과*

A new functionalized macrocycle 2,13-bis(phenacyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (B) bearing two *N*-phenacyl pendant arms has been prepared by the reaction of 3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (A) with 2-bromoacetophenone. Its copper(II) and nickel(II) complexes have been prepared and characterized. The phenacyl groups of $[Ni(B)]^{2+}$ and $[Cu(B)]^{2+}$ are coordinated to the metal ion in the solid state and in various solvents. In basic aqueous solutions, the complexes undergo tautomerization and deprotonation to form neutral complexes where the functional pendant arms are coordinated to the metal ion as its enolate form. Synthesis and chemical properties of the compounds are presented, along with the crystal structure of $[Ni(B)]^{2+}$.

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장소: 대구엑스코
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Template Synthesis of 15-Membered Hexaaza Macrobicyclic and Macrotricyclic Copper(II) Complexes

강신걸, 김현자, *정수경

*대구대 화학과 *김포대학 호텔조리학과*

The hexaaza macrobicyclic copper(II) complex $[Cu(A)]^{2+}$ (A = 6-methyl-9-methoxymethyl-1,3,6,9,11,14-hexaazabicyclo[12.2.1]heptadecane) has been prepared by the metal-template condensation of formaldehyde with diethylenetriamine and 4-methyl-1,4,7-heptane in methanol. In $[Cu(A)]^{2+}$, the macrobicyclic ligand containing one 1,3-diazacyclopentane ring is coordinated to the metal ion with a 5-6-5-7 chelate ring sequence. The complex is rapidly decomposed in acidic aqueous solution. Although the complex is relatively stable in pure water at room temperature, it is hydrolyzed to $[Cu(B)]^{2+}$ (B = a non-macrocyclic hexamine) at an elevated temperature. The metal-directed condensation of formaldehyde with 1,5,9,13-hexaazatridecane, ethylenediamine, and formaldehyde produces $[Cu(C)]^{2+}$ (C = 1,3,6,8,12,16-hexaazatricyclo[14.3.1.1$^{8.12}$]heneicosane) with a 5-6-6-6 chelate ring sequence. This complex is much more inert against decomposition than $[Cu(A)]^{2+}$. Synthesis and chemical properties of the copper(II) complexes are presented.

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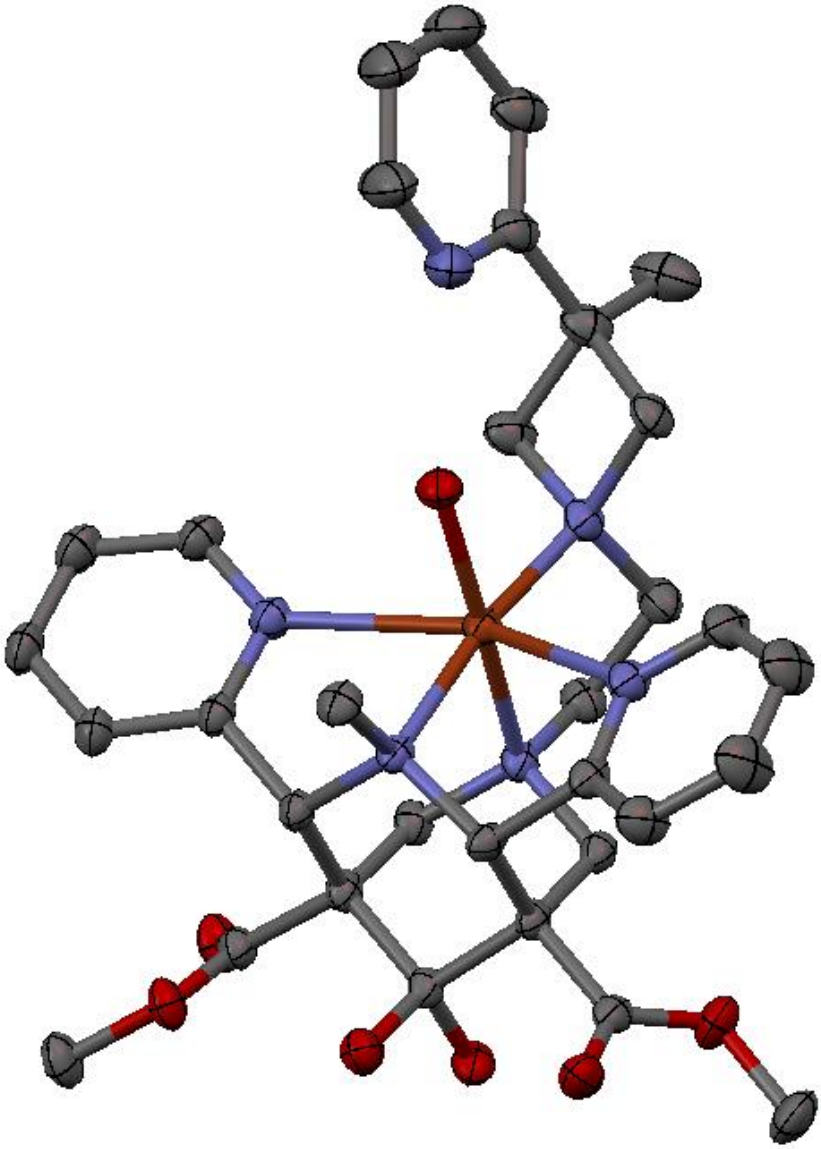
발표코드: **INOR.P-15**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Multidentate Ligands and Their Complexes of Small-ring Heterocycles

신디, *김미현, 김양, *조정환, **변종철, ***최지영, ****이경렬

*고신대 화학 신소재학과 *고신대 화학신소재학과 **제주대 자연과학대학 화학과 ***제주대 화학과 ****성지고 연구기획부*

The synthetic utility of three- and four-membered heterocyclic rings as molecular constituents is in large part due to the facility of their ring opening reactions. This reactivity can be usefully controlled by metal ion binding to the heteroatom, although any influence that metal ion binding may have when the heteroatom is not directly bound and the ring is simply part of the superstructure of a multidentate ligand is less clear. As part of our studies of the synthesis and applications of azetidine-derived ligands, we present herein some structural studies bearing on these issues.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-16**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Construction of Cd(II) Complexes with a 2,2'-Dipyridiylamine (Hdpa): Anion Effect and Catalytic Activities

김진훈, *송영주, *장승표, *김철, **김영미, ***김성진

*서울산업대 생무기연구실 *서울산업대 정밀화학과 친환경소재제품센터 **이화여대 화학-나노과학과 ***이화여대 화학과*

Six new structures of Cd(II) complexes with chelating ligands (Hdpa) have been characterized. 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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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Light-Induced Self-Assemblies Suitable for Photodimerization and Their Light-Induced Solid-State [2 + 2] Cycloaddition in Solution

박현민, *이정아, **김진훈, 이홍규, 조영단, ***김철, ****김성진, *****김영미

*서울산업대 정밀화학과 *서울산업대학원 정밀화학과 **서울산업대 생무기연구실 ***서울산업대 정밀화학과 친환경소재제품센터 ****이화여대 화학과 *****이화여대 화학-나노과학과*

The reaction of Cd(NO3)2 and CF3COONH4 with bpe ligands has been investigated for the light-induced solid-state [2 + 2] cycloaddition reaction in solution. The light has affected the construction of three different compounds, and their structures show both parallel and criss-cross alignments of C=C olefin bonds to satisfy for the Schmidt's geometric criteria for the solid-state photochemical [2 + 2] cycloaddition reaction. All three compounds have been completely transformed to the final cycloaddition products containing rctt-tpcb although only one structure among them has been determined. Besides X-ray and NMR, moreover, the fluorescence allowed us to monitor the progress of the solid state reaction and was found to be a valuable tool. In addition, the complexes 1 and 3 exhibit fluorescence emission bands at ca. 417 nm, indicating that 1 and 3 may be excellent candidates for potential photoactive materials. Furthermore, 1, 3, and 4 showed an efficient catalytic transesterification reaction with vinyl acetate.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel chains constructed from heterotrinuclear units and 1,2-bis(4-pyridyl)ethane formulated as [M2M'(O2CPh)6](bpa) (M = Co, Zn, M' = Co, Cd) : their catalytic activity

이홍규, *이정아, 조영단, **김철, ***김성진, ****김영미

*서울산업대 정밀화학과 *서울산업대학원 정밀화학과 **서울산업대 정밀화학과 친환경소재제품센터 ***이화여대 화학과 ****이화여대 화학-나노과학과*

Three novel heterometallic complexes containing two bridging ligands bpa and benzoate, formulated as [M2M'(O2CC6H5]n(bpa)n (bpa = 1,2-bis(4-pyridyl)ethane, M2M' = Zn2Co (1), Zn2Cd (2), and Co2Cd (3)), have been synthesized. All three compounds show one-dimensional structures containing linear heteronuclear coordination units linked by bridging bpa ligands. Reactivity study of the compounds 1 - 3 for the transesterification of a variety of esters has shown that they are very efficient and 2 is the best among them.

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발표코드: **INOR.P-19**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Amide-Based Nonheme Manganese(III) Hydrocarbon Oxidation Catalysts: Involvement of Multiple Active Oxidants and the Generation of the MnV=O Species as the Dominant Oxidant

송영주, 장승표, *박현민, 김철

*서울산업대 정밀화학과 친환경소재제품센터 *서울산업대 정밀화학과*

Mononuclear nonheme manganese(III) complexes, [Mn(bpc)Cl(H2O)] (1) and [Mn(Me2bpb)Cl(H2O)]CH3OH (2), were prepared and characterized. Complex 2 has also been characterized by X-ray crystallography. Magnetic measurements revealed that the complexes are high spin (S=5/2) MnIII species with typical magnetic moments of 4.76 and 4.95 ´ B, respectively. These nonheme MnIII complexes efficiently catalyzed olefin epoxidation and alcohol oxidation upon treatment with MCPBA under mild experimental conditions. Olefin epoxidation by these catalysts is proposed to involve the multiple active oxidants MnV=O, MnIV=O, and MnIII-OO(O)CR. Evidence for this approach was derived from reactivity and Hammett studies, KIE (kH/kD) values, H218O-exchange experiments, and the use of peroxyphenylacetic acid as a mechanistic probe. In addition, it has been observed that the participation of MnV=O, MnIV=O, and MnIII-OOR can be controlled by changing the substrate concentration. Moreover, partitioning between heterolysis and homolysis of the O-O bond of a Mn-acylperoxo intermediate (Mn-OOC(O)R) was significantly affected by the nature of solvent, and the O-O bond of the Mn-OOC(O)R proceeded predominantly by heterolytic cleavage in protic solvent. Therefore, a discrete MnV=O intermediate appeared to be the dominant reactive species in protic solvent. Furthermore, we have observed close similarities between these nonheme MnIII complex systems and Mn(saloph) catalysts previously reported, indicating that this simultaneous operation of the three active oxidants might prevail in all the manganese-catalyzed olefin epoxidations, including Mn(salen), Mn(nonheme), and even Mn(porphyrin) complexes.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of silica@coordination polymer core-shell structures and their utilization

조치호, 오문현

연세대 화학과

Recently, the hollow micro- and nano-structures have been extensively studied due to their useful properties and applications such as drug-delivery carrier, nanoscale chemical reactor, catalyst and photonic building block. Herein, we present the preparation method for the silica@coordination polymer core-shell structures with controlled shell thickness. A novel approach in the utilization of the core-shell structures of silica@coordination polymer as precursors for the preparation of the core-shell structures of silica@metal oxides and the hollow metal oxides with tunable thickness has been also developed.

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발표코드: **INOR.P-21**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Utilization of coordination polymer particles (CPPs) for the selective preparation of hematite and magnetite nano-rods

박승진, 조원, 오문현

연세대 화학과

Iron oxide particles have been widely studied due to their unique properties and resulting many useful applications. Among them, the hematite (α-Fe_2O_3) has been utilized as gas sensor, catalyst and electrode material. Magnetite (Fe_3O_4) has been used in many biomedical areas such as magnetic resonance imaging (MRI) contrast agent. Herein we report a novel methodology for the selective preparation of hematite and magnetite particles from coordination polymer particles (CPPs). A rod-shaped CPP can be selectively transformed to a hematite or magnetite nano-rod depending upon the reaction conditions.

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New n-type low bandgap conjugated polymer of structural and electronic properties

송주만, 최현봉, 고재중

고려대 소재화학과

Bandgap and molecular energy level control are great important in improving photovoltaic properties of conjugated polymer. A common approach to tuning these parameters is to modify the structure of conjugated polymers by co-polymerizing with different unit. We made a n-type low bandgap conjugated polymer based on new structure of perylene diimide and benzodithiophene, which exhibits excellent reversible electrochemical properties, was designed, synthesized and characterized.

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High efficiency dye-sensitized solar cells with an organic chromophore featuring a π-conjugated spacer

도광석, 정반석, 김주영, 김철우, 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. JK-190 and JK-191 containing long alkyl chain attached fused-amine for donor group are designed and synthesized. Under standard global AM 1.5 solar condition, We found that the η of JK-190 was higher than η of JK-191 due to the higher Voc and Jsc. The improved Voc and Jsc value is attributed to the suppression of dark current owing to the blocking effect of a long alkyl chain at donor. By introducing electron-rich biEDOT units, the light absorptions as well as photocurrent spectral responses of dye have been remarkably red-shifted.

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A new class of organic sensitizers with fused planar triphenylamine for nanocrystalline dye sensitized solar cells

김철우, 최현봉, 백상현, *송기형, 고재중

*고려대 소재화학과 *한국교원대 화학과*

Five novel organic sensitizers that contain a fused-planar triphenylamine as electron donor have been synthesized and their photophysical properties, theoretical calculation and photovoltaic performances as well as stability test have been studied. Under standard AM 1.5 sunlight, the sensitizer JK-164 yielded a short-circuit photocurrent density of 15.32 mA cm-2, an open-circuit voltage of 0.70 V, and a fill factor of 0.74, corresponding to an overall conversion efficiency of 7.86%. The JK-164 cell exhibits an excellent stability, revealing a slight change after 1000 h of light soaking at 60 °C using a solvent free ionic liquid. The cell shows a higher open-circuit voltage (Voc) compared to that of JK-163 due to an increased electron life time (τc) in the conduction band of TiO2.

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Soluble Triisopropylsilylethynyl Anthracene Derivatives for Organic Photovoltaic Cells

최혜주, 김주영, 송주만, 김철우, 백상현, 고재중

고려대 소재화학과

Organic solar cells based on organic semiconductors are currently attracting a growing interest worldwide. One essential reason for that is the possibility to realize flexible and low-cost photovoltaic (PV) cells by taking advantage of the easy processability of organic matter at relatively low temperatures. Anthracene based semiconductors have been investigated by several serearch groups, because they have higher oxidative stability than that found for pentacene. We introduce anthracene derivatives containing heteroaromatic derivatives and electron-withdrawing group at the 2,6 positions of TIPSAnt core for the solubility and crystallinity. We expect to the introduction of electron-acceptor group induces an extension of the photoresponse in the visible spectral region.

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A new class of cyclometalated ruthenium sensitizers for efficient dye sensitized solar cells

최현봉, 백상현, 임기민, 고재중

고려대 소재화학과

Dye-sensitized solar cells(DSSCs) based on nanocrystalline semiconductor have been intensively studied because of their potential low-cost, easy processing and high performance. a new class of cyclometalated ruthenium sensitizers JK-206 and JK-207 were meticulously designed and synthesized. The photovoltaic performance of JK-206 is superior to the N719. Moreover, the JK-206 device showed an excellent stability under light soaking at 60 oC for 1000 h. The high efficiency and excellent stability may be attributed to the intrinsic stability of cyclometalated ruthenium complex with C^N^N ligand, and the broad and red-shifted absorption pro-perty of the cyclometalated complex.

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Efficient and stable panchromatic squaraine near-IR dye for dye-sensitized solar cells

백상현, 최현봉, 김철우, 조나라, 고혜민, 고재중

고려대 소재화학과

Dye-sensitized solar cells(DSSCs) based on nanocrystalline semiconductor have been intensively studied because of their potential low-cost, easy processing and high performance. A new series of stable, unsymmetrical squaraine near-IR sensitizers (JK-216 and JK-217), which are assem-bled using both thiophenyl pyrrolyl and indolium groups, exhibit a panchromatic light harvesting up to 780 nm. The JK-216 based cell exhibited a record efficiency of 6.29% for near-IR DSSCs. In addition, the JK-126 device showed an excellent stability under light soaking test at 60 oC for 1000 h. The interesting new result is that the device can be applicable to a possible use of “photovoltaic windows” for green house or BIPV.

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Organic Sensitiser Containing Perylene derivatives for Efficient Panchromatic DSSCs

김경준, 고혜민, 김철우, 최현봉, 고재중

고려대 소재화학과

Molecular photovoltaic devices with extended absorption in the near-IR region of the spectrum are currently a hot topic in the area of solar cells. As metal-free dyes, perylene derivatives have been widely applied in various optical devices owing to their outstanding chemical, thermal and photochemical stability and non-toxicity. Several perylene dyes have been used as sensitizers in DSSCs, however, they exhibited very low overall power conversion efficiencies (η=1~2%). For that reason, we introduced organic dye that consist of the bis-dimethylfluoreneaniline moiety acting as electron donor and the two functions being connected by conducting thiophene units.

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Introduction of the pyrrole chromophores as π-bridge of organic dyes

최홍식, 김철우, 소슬기, 최혜주, 송주만, 고재중

고려대 소재화학과

The sensitizer is a critical component in nanocrystalline dye sensitized solar cells (DSCs) that have great potential for future photovoltaic applications owing to their high efficiency and low production cost. In this study, two organic dyes have been designed and synthesized. The heterocycle moieties on the bridge of the organic dyes were varied as to be bis(1-n-hexylpyrrole) and ter(1-n-hexylpyrrole). The properties of the two new molecules were comparatively studied. We could find trend according to increase number of pyrrole moieties. In addition, these results are critically analyzed along with a prepared compound, reported earlier from our laboratories, that contain bis(thiophene) as bridge, keeping the donor and the acceptor.

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Trifluoropropenyl as spacer group of organic sensitizer for DSSC

유태정, *김철우, *최혜주, *김주영, *송주만, *조나라, *고재중

*고려대 신소재화학과 *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 designed organic sensitizer containing Trifluoropropenylbenzene moiety as bridge group. As the introduction of Trifluoropropenylbenzene moiety into bridge group, we expect to increase π-conjugation and prevent aggregation. Consequently, we obtained new organic sensitizer having good power conversion efficiency .

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Molecular Engineering of Diketopyrrolopyrrole-Based Photosensitizer for Solution Processed Small Molecule Bulk Heterojunction Solar Cells

정반석, 조나라, 송주만, 김철우, 고재중

고려대 소재화학과

The synthesis and characterization of the novel derivatives, DPP-bis[HT3-TPA] of DPP-thiophene with triphenylamine (TPA) end group for BHJ solar cells utilizing a BHJ active layer consisting of small molecule as a donor and PCBM as acceptor were demonstrated. The molecular engineering of DPP core based photosensitizer with TPA were used for stabilizing the separated hole from exciton and improving the transporting property of hole carrier and the band-shift by more efficient intramolecular charge transfer for high-efficiency BHJ device. The most efficient devices, obtained using DPP-bis[HT3-TPA]/C_{71}-PCBM BHJ film, after post-annealed at 100˚C for 5 min had an average power-conversion efficiency of 1.5% under 100mW/cm^2, with short-circuit current J_{sc} = 5.73 mA/cm^2, fill factor FF = 0.45, and open-circuit voltage V_{oc} = 0.59 V; i.e. ~13% higher efficiency than obtained without post-annealing process. The DPP-bis[HT3-TPA] based BHJ device exhibits below 0.6 V of low V_{oc} caused by the TPA donating effect that can rise the HOMO level of molecule, with giving an important guide for developing new materials in solution-processed small molecule BHJ solar cell.

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Small-Molecule Bulk Heterojunction Solar Cells Based on Near-IR Dyes

소슬기, 최홍식, 최혜주, 김경준, 김철우, 고재중

고려대 소재화학과

Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. We attempted that polymer p-type donor was to be replaced by small-molecule p-type donor. Solution processable small-molecule-based BHJ solar cells are becoming increasingly attractive because it is possible to simple purification and accessibility.We made two unsymetrical squarain dyes, JK-209 and JK-210, contacting 3-hexylthiophenes and 1-hexylpyrrole. They exhibit sharp and intense absorption band in the near infrared (NIR) spectral region. The solution-UV spectra exhibits typical squarain absorptions at 696nm and second absorbance bands with a maximum at 400 nm, the film-UV spectra is broad and span the 350～840 nm region. The HOMO and LUMO energies of both molecules estimated by cyclic voltammetry are -3.4 and -5.0 eV.

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Magnetic Triggering of Intracellular Signaling: Implication on the Angiogenesis Control

조미현, 이재현, *손민아, **신전수, 천진우

*연세대 화학과 *연세대 나노메디컬학과 **연세대 의과대학 미생물학교실*

Artificial control of cellular activities is of high interest in biomedical sciences. The activation of receptors on the cells is typically driven by biochemical ligands, but nanoscale tools can also perform such a role. Here, we report nanoscale-magneto-activated cellular signaling (N-MACS) for receptor mediated angiogenesis which is a vital process related to blood vessels and cancer metastasis. Target specific antibody and magnetic nanoparticle conjugates, which are first bound to Tie2 receptors on cell surfaces, are clustered by translational forces exerted through external magnetic field. Such mechano-cell activations are confirmed by identifying down-stream cell signaling signatures including phosphorylations of Tie2, Akt, and reactive oxygen species. This phenomenon serves as a “trigger-on” for a number of Tie2 related intracellular signaling events that cause human umbilical vein endothelial cells (HUVEC) to undergo tubulogenesis, which is the pre-angiogenesis stage. Our results suggest that vascular-specific cellular activities can be controlled in a remote and precise fashion via molecular-level N-MACS approach.

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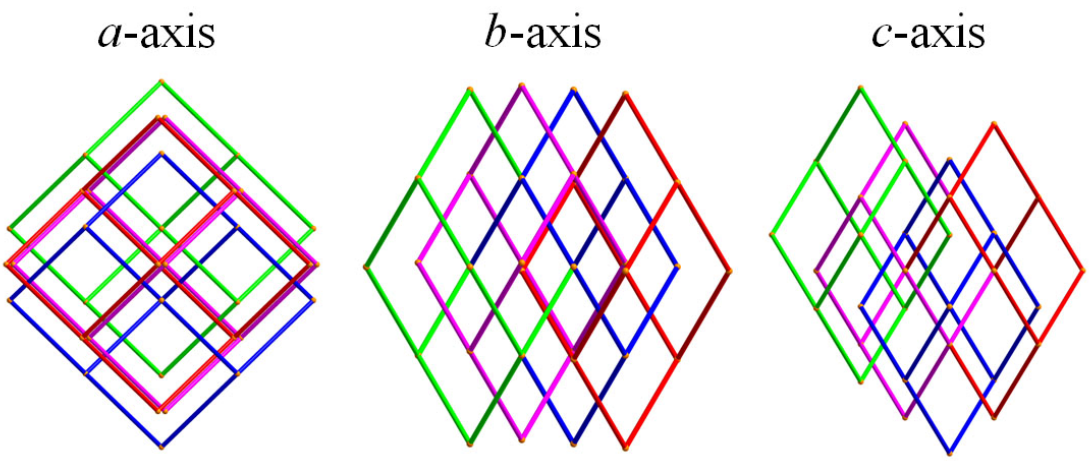
4-Fold Interpenetrated Diamond Network of In-MOF Containing 4,4'-Biphenyldicarboxylate Bridging Ligands

허성, 구자민, *김성진, **김영미

*한국외국어대 화학과 *이화여대 화학과 **이화여대 화학-나노과학과*

In pursuit of new topologically interesting high surface metal-organic frameworks (MOFs), we prepared In-MOFs using a 4,4'-biphenyldicarboxylate (BPDC) bridging ligand. The In-MOFs were characterized by X-ray crystallography, powder X-ray diffraction, TGA, and gas sorption analysis. One form of this system, isomer A, showed a 3-dimensional (3D) diamond-like 6^6 topology. There are two crystallographically independent In(III) centers. Each frameworks interpenetrates doubly with $Z_t = 1$, $Z_n = 2$, $Z = 2$, and the class is IIa. Therefore, the whole frameworks exhibit overall 4-fold interpenetration. The Schläfli symbol of the each In(III) atom is 6^6-dia. PLATON analysis indicates that the solvent accessible void without solvent molecules is 58.4%. We also prepared another structure, isomer B, under different conditions which showed doubly interpenetrated 3D network. Isomers A and B are unusual catenation isomers. Gas sorption analysis will also be presented.



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Guest-Free Structures of a Metal-Organic Framework Depending on Activation Methods and Temperature

박혜정, *임대운, 백명현

*서울대 화학부 *서울대 화학과*

We demonstrate by the complete single crystal X-ray diffraction analyses how the guest-free structure of a Zn_4O-based MOF depends on the activation methods such as room temperature evacuation, supercritical CO_2 treatment, and high temperature evacuation. We also reveal by the variable temperature synchrotron X-ray single crystal diffraction studies that the temperature induces structural transformation of a guest-free MOF. The guest-free MOFs prepared by different activation methods exhibit different fine structures at room temperature, having different effective window sizes and window shapes.

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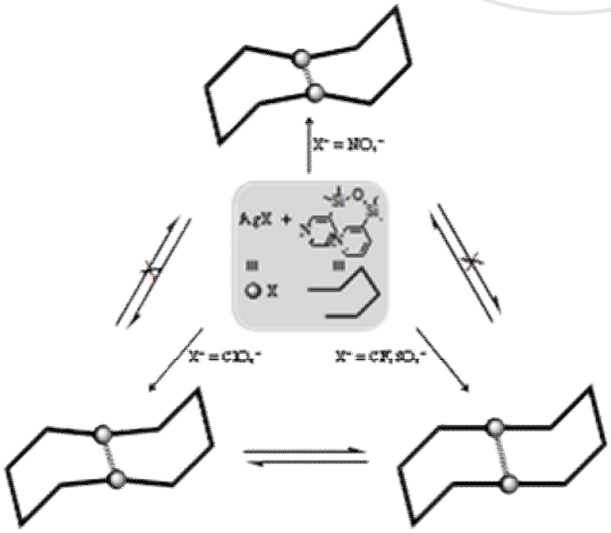
Fine competition and control among argentophilic, electrostatic, and π···π interactions in a metallacyclodimer

안정민, 정옥상

부산대 화학과

The reaction of AgX (X^- = NO_3^-, ClO_4^-, and $CF_3SO_3^-$) with 1,3-bis(3-pyridyl)tetramethyldisiloxane (L) at room temperature affords 20-membered metallacyclodimers, $[Ag(L)]_2(X)_2$. For the macrocyclodimer, fine competition among argentophilic, electrostatic, and π···π interaction exists. The macrocyclodimer is a unique molecular chair that tunes a transannular argentophilic interaction via the bite size of counteranions. In order to reversibly control the argentophilic interaction, anion exchange has been accomplished. The anion exchangeability is depending on the water-solubility rather than the electrostatic interaction between silver(I) and anions.



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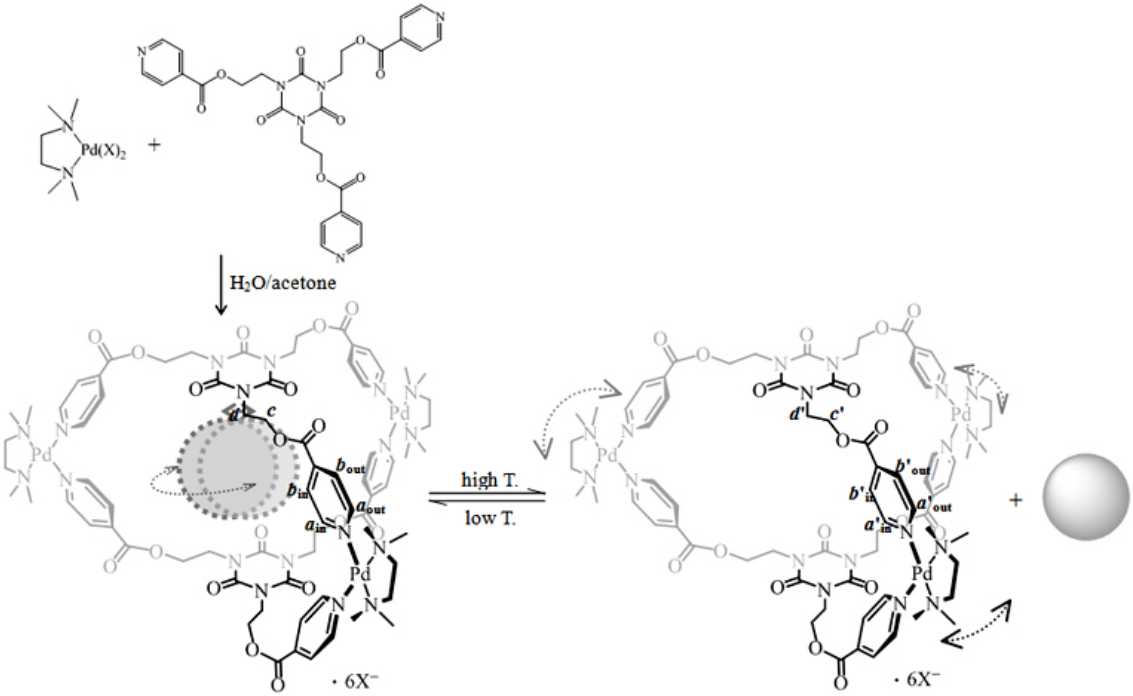
Tractable Behavior of an Isolated Water Molecule within a Small Cage

노태환, 정옥상

부산대 화학과

Research on a single water molecule including interaction with and isolation from a host is an important issue in molecular science owing to the precise function of proton transfer, tautomerism, and biological system. In particular, the discrete water clusters such as tetramer, pentamer, hexamer, octamer, and decamer have been known to exist within crystalline hosts through hydrogen bonds because of its fundamental importance. In this work, to validate the concept and chemistry for the formation of cage containing a flexible tridentate ligand, we report a cage, $[Pd_3L_2]^{6+}$ (Pd = $(Me_2en)Pd(II)$) via construction of a new C_3-symmetric potential triangular component with *cis*-protected ditopic $(Me_2en)Pd(II)$ as a corner linker. A single water molecule is nestled within the new cage, and is reversibly adsorbed and desorbed via the process of a noncovalently bound complex. Thus, the duality of liberal and restrictive properties of a single water molecule has been discussed based on spectroscopic data. To date, no research on a single water molecule within a cage compound without significant interactions has been published.



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Lower-Critical-Solution-Temperature Behavior and Catalytic Effects via Labile Bonding Modes of Bimetallic (Diallylmalonato)platinum(II) Complexes

김치원, 정옥상

부산대 화학과

The ability to reversibly modulate structures and physicochemical properties by means of chemical triggers is of central importance in the development of molecular switching materials. The process of transition metal complex interconversion offers some potential to the design of various molecular materials including memory and storage materials, sensors, and logic systems. Research on the lower critical solution temperature (LCST) at which phase separation above a critical temperature occurs has attracted much attention owing to applications such as drug delivery systems, catalysis and synthesis supports, and separation. To date, reports of interest on LCST materials have been limited to discotic organic compounds and organic polymers. As such, the LCST behavior of designed discrete metal complexes remains unexplored. In order to determine the thermoresponsive properties of transition metal complexes containing a non-innocent ligand, here report on the stepwise syntheses, LCST behaviors, and catalytic properties of bimetallic (diallylmalonato)platinum(II) complexes. No research results on the direct catalytic effects on LCST materials have yet been disseminated. Several years ago, it was reported that the bonding nature of the diallylmalonate ligand (L) is subtly determined by various factors such as coligands, solvents, and temperature. The nature of the coordination of potential multidentate L will prove useful to the design and synthesis of bimetallic platinum(II) complexes via the “metalloligand” concept, an important synthetic strategy for achieving polymetallic molecular structures. In fact, various platinum species have been widely used as catalysts in chemical reactions.

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Hexagonal Nanodiscs of CuSe Synthesized through a Solution Phase Reaction

Jin Xing, 김진권

공주대 화학과

Copper selenides are p-type semiconductors having potential applications in solar cells, optical filters, nanoswitches, thermoelectric and photoelectric transformers and superconductors. Synthesis of CuSe nanomaterials in various morphologies has attracted much attention due to their physicochemical properties and applicability. Herein we present a novel solution-phase synthetic route for obtaining hexagonally shaped nanoplatelets of copper selenide. Chemical reaction involved in the synthesis is the reduction of copper selenite ($CuSeO_3$) with hydrazine hydrate. The reaction is performed in various solvents and in presence of different capping agents. The structure, composition and properties of the nanomaterials obtained were studied with various techniques. The reduction reaction carried out in ethylene glycol even in the absence of any capping agents gave the best results. The relatively low temperature of reaction, usage of single precursor and the surfactant-free growth of nanomaterials make this synthetic route a promising one in perspectives of material science and nanochemistry.

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Part III-Dinuclear Ni(II) pseudohalogen complexes containing a bridged thienylene ligand

김용주, 이혁희, 이정현, *장영옥, *이순원

*강릉대 화학과 *성균관대 화학과*

Dinuclear Ni(II) halogen complexes containing a bridged thienylene ligand are prepared from oxidative addition of dihalothienylene compounds to a Ni(0) complex. Sequential treatments with NaN3 to the dinuclear Ni(II) halides cause the corresponding dinuclear azido complexes in high yields and then chemical reactivities toward organic unsaturated compounds such as TMS-NCS and TMS-CN have been examined.

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Preparation of Chiral Tetrazole-thiolato Pd(II) and-Pt(II) complexes and their relevant organic reactions

김용주, 이혁희, 한삼용, 경영수, *이경은, *장영옥, *이순원

*강릉대 화학과 *성균관대 화학과*

Bis(azido)Pd(II) or -Pt(II) complexes reacted with chiral isothiocyanates(R-NCS) to give corresponding chiral tetrazole-thiolato Pd(II) and -Pt(II) complexes. Isolated complexes were determined by spectroscopic and X-ray diffraction studies. Reactivites toward some electrophiles such as HCl or benzolyl chlorides produced heterocyclic compounds containing a tetrazole thione or a tetrazolyl sulfide group. In particular, various organic tetrazole thiones, 1-alkyl(or aryl)-1H-tetrazole-5(4H)-thiones containing a chiral moiety, were prepared from NaN3 and organic isothiocyanates in the presence of water. On the other hand, 5-substituted thiatriazoles were selectively prepared in THF and HCl media.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Silver and Palladium Complexes with New N-Heterocyclic Carbene Ligands

정현진, 이문선, 배호연, *박경세, 이동헌

*전북대 화학과 *군산대 화학과*

Silver N-heterocycle carbene(NHC) complexes have recently been highlighted as promising reagents for potential anticancer and antimicrobial agents, catalytic reagents and so on. Silver NHC complexes are also very useful precursors for NHC complexes of other metals. Here we report on the syntheses and characterization of silver(I) and palladium(II) complexes containing pyridine substituted NHC ligands. The two new silver complexes were synthesized by the treatment of N-heterocyclic chelates, 1,3-bis[(6-methyl-2-pyridyl)methyl]imidazolium bromide and 1,3-bis[(6-methyl-2-pyridyl)] imidazolium bromide with Ag_2O, respectively. Palladium complexes were obtained from the silver complexes by the transmetalation reactions with $PdCl_2(CH_3CN)_2$. The molecular structures of the complexes have been elucidated by single-crystal X-ray crystallography. We also examined the Heck coupling of bromobenzene and styrene using one of the palladium complex as a catalyst.

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Synthesis and Characterization of New ^{188}Re, ^{99m}Tc complexes for Molecular Imaging Agent

양민규, *박상현, **이효선

*경북대 화학과 *한국원자력연구원 방사선생명공학연구부 **경북대 자연과학대학 화학과*

Apoptosis plays an important role in normal tissue homeostasis and in pathogenesis of numerous medical disorders. The clinical molecular imaging of this process may enhance diagnosis, efficiency of treatment, and monitoring of disease. We intended to synthesize new molecular imaging substrate system based on original ML-10 with the modification of fluoride moiety with several new tridentate ligands e.g. 2-[(pyridin-2-ylmethylene)-amino]-phenol, bis-pyridin-2-ylmethyl-amine, and carboxymethyl-amine. The synthesized ligand systems are capable of coordination with radioactive metals e.g. ^{188}Re, ^{99m}Tc . Thus, the radioactive nature of the metal in the synthesized complexes can be utilized in clinical molecular imaging for monitoring the cancer affected cell response to treatment and the efficiency of treatment as these compounds respond to the alteration in plasma membrane potential. Furthermore, the emission of β-rays of complexes are capable to cure cancer cell directly.

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Organosilver Complexes Synthesized by Ultrasonic Treatment for the Potential Applications of Silver Paste and Inks

구자민, *이효선

*경북대 화학과 *경북대 자연과학대학 화학과*

Printable conducting materials such as conductive inks and pastes are inevitable for electronics industry. Commercially, silver pastes composed of mainly silver oxide and silver salt of carboxylic acid, are applied to the printed transistor circuits with suitable process, i.e. thermal reduction. This process presumably can be substituted for electron beam that brings a simplification of process, economical, environmental friendly process and pave a way to the development of flexible substrate. However, the use of electron beam for synthesis of organosilver complexes is limited because of their poor solubility. We are going to use the ultrasonic treatment as thermal source for the syntheses of organometallic complexes such as silver, copper, nickel and palladium based on tripodal amine ligands. The synthesis of new amine based on ligand system e.g. tris(hydroxymethyl)amine, tris(chloromethyl)amine, tris(hydroxycarbonylmethyl)amine, and tris-pyrazol-1-ylmethyl-amine and their complexation to Ag, and Cu metals have been carried out successfully. All complexes were synthesized in high yield and purity and fully characterized by various spectroscopic techniques. The new complexes were utilized for conductive paste and inks in company with the method of reduction by electron beam treatment.

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Novel Alkylidene Ruthenium Complex Systems for Ring-Opening Metathesis Polymerization of Functional Cyclic Olefins

우현율, *성익경, **이효선

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

The development of well-defined ruthenium-based complexes capable of catalyzing olefin metathesis, has been particularly focused due to their increased tolerance to functional group in the substrate. However, synthesis of the first generation Grubb's Ru catalyst is very painful with low yield due to rapid decomposition of diazomethylbenzene intermediate. Also, second generation Grubb's Ru catalyst is very expensive. In this study, highly activated catalyst systems for the ROMP of functional strained olefins are readily prepared from the most stable intermediate (INT) of Grubb's 1st generation catalyst by the alkylidene exchange reaction with olefinic substrates such as (1-methyl-3-vinylimidazolium iodide, 1-methyl-4-vinylpyridinium iodide and vinylpyrrole). In addition, we focused on the synthesis of ligand system (E)-N-((1H-pyrrol-2-yl)methylene)-2-isopropoxyaniline) [Npmpa] and (E)-N-((3,5-dimethyl-1H-pyrazol-1-yl)(phenyl)methylene)-2,6-diisopropylaniline [Ndppm] and their complexation to Ru-metal, to make new efficient ROMP catalyst for cyclic olefins.

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Structure, Spectroscopy and Ligand Field Analysis of *trans*-$[Cr(Me_2tn)_2Cl_2]_2ZnCl_4$

최종하, 오세영, *유건상, **이상학

*안동대 화학과 *안동대 응용화학과 **경북대 화학과*

The structure of *trans*-$[Cr(Me_2tn)_2Cl_2]_2ZnCl_4$($Me_2tn$ = 2,2-dimethylpropane-1,3-diamine) has been determined by a single-crystal X-ray diffraction study at 173 K. The analysis reveals that there are three crystallographically independent Cr(III) complex cations in the title compound. The Cr(III) atoms are coordinated by four N atoms of Me2tn and two chlorine atoms in trans arrangement, displaying a distorted octahedral geometry. The orientations of two six-membered chelate rings in three complex cations are in anti chair-chair conformation with respect to each other. The Cr–N and Cr–Cl bond lengths average 2.0862(2) and 2.3112(6) Å, respectively. The $ZnCl_4^{2-}$ have slightly distorted tetrahedral geometry with Zn–Cl lengths and the Cl–Zn-Cl angles influenced by hydrogen bonding. The resolved absorption maxima in the electronic d-d spectrum were fitted with a secular determinant for a quartet energy state of the d3 configuration in a tetragonal field. It is confirmed that the nitrogen atoms of the Me2tn ligand are strong σ-donors, but the chloro ligands have weak σ- and π-donor properties toward the chromium(III) ion.

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Synthesis and Structure of Diaqua(5,16-dimethyl-2,6,13,17-tetraazatricyclo[14,4,$0^{1,18}$,$0^{7,12}$]docosane)copper(II) Bis(tetrafluoroborate) Dihydrate

최종하, 오세영, *이상학, **유건상

*안동대 화학과 *경북대 화학과 **안동대 응용화학과*

The newly synthesized complex salt crystallizes in the space group $P2_1/n$ of the monoclinic system with two mononuclear formula units in a cell of dimensions a = 8.9327(1), b = 18.3628(3), c = 8.9811(2) Å and β = 100.665(1)^o. The copper(II) ion with 5,16-dimethyl-2,6,13,17-tetraazatricyclo(14,4,$0^{1,18}$,$0^{7,12}$)docosane (L^1) has a tetragonally distorted octahedral environment with the four N atoms of the macrocyclic ligand in equatorial positions and the O atoms of two water molecules in axial positions. The macrocyclic ligand adopts the most stable trans-III conformation. The Cu-N distance of 2.028(2) Å is normal, but the elongation of Cu-OH_2 bond, 2.693(3) Å may be due to the peudo Jahn-Teller effect and the strong in-plane ligand field. The crystal is stabilized by a three-dimensional network of hydrogen bonds among secondary N hydrogens, F atoms of BF_4^- and O atoms of water molecules.

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Crystal Structure and Spectroscopic Properties of Zinc(II) Complexes with Constrained Macrocyclic Ligands

최종하

안동대 화학과

Four novel zinc(II) complexes with Hexyl-Me2-cyclam (L1) 3, 5 and Naphthyl-hexyl-Me2-cyclam (L3) 4, 6 were have synthesized. Complexes with both three and four nitrogens from the macrocyclic ring bound to zinc centers were observed and X-ray crystal structures were determined for complexes 3 and 6. Crystallographic data for 3 shows the zinc complex is six-coordinate in a distorted octahedral environment by four N atoms from the macrocyclic ligand in equatorial positions and two O atoms of acetato groups in axial positions. The 14-membered metallo-macrocycle adopts a trans-III (RRSS) configuration with two six-membered rings in chair forms and two five-membered rings in gauche forms. For chlorido complexes the zinc centre in the 4N-bound species 5 appears to be 5-coordinate and most likely adopts a square-pyramidal geometry. Interestingly, complex 6 crystallized in a trans-I configuration containing a 4-coordinate tetrahedral zinc centre to three of the ring nitrogen atoms and may show a possible intermediate in the mechanism for uptake and release of metals by cyclams. In terms of the relationship between metal-carboxylate binding and anti-HIV activity, the acetato complexes were tested. The effect on configurational change for different axial ligands was investigated using 2D [1H, 13C] and [1H, 15N] solution NMR spectroscopy.

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Cu_2O Nanocubes Catalyzed Difunctionalization Reaction of Vinyl Arenes with Cyclic Ethers

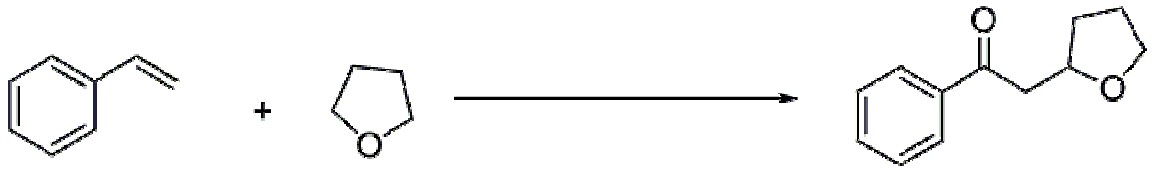
허은정, 김지영, 박강현, *박지찬, *송현준

*부산대 화학과 *KAIST 화학과*

Metal nanoparticles whose sizes are between those of bulk and monomeric metal species have a wide range of applications; such nanoparticles are used in various electronic, optical, and magnetic devices as well as in the production of catalytic materials. Transition-metal nanoparticles are an important class of catalysts used in organic synthesis. In recent years, significant improvements have been made to transition-metal-catalyzed C-C and C-H bond formation reactions. In particular, functionalization of arenes via transition-metal catalysis, i.e., conversion of arenes to more valuable derivatives, has been identified as a very important reaction that can revolutionize the chemical industry.

Extensive studies have been carried on the use of copper in organic synthesis because copper is a promising candidate for a highly efficient catalyst. Recently, remarkable improvements have been made to various copper-nanoparticle-catalyzed reactions such as the Ullmann reaction, click reaction, cross-coupling reactions, cyclization reactions, oxidation, and oxyalkylation. We have recently identified a very attractive alternative synthetic route to biaryl ethers. This synthetic route involves the reaction of an aryl halide with a phenol in the presence of Cu_2O nanocubes. This process is simple and allows the formation of a diverse range of biaryl ethers in excellent yields. Another important advantage of this synthesis method is that the catalyst can be easily recycled without loss of activity and used as such without further purification.

Herein, we report a novel difunctionalization of vinyl arenes; in this reaction, well-designed, uniform Cu_2O nanoparticles are used to catalyze the regioselective oxyalkylation of vinyl arenes under mild conditions.



대한화학회
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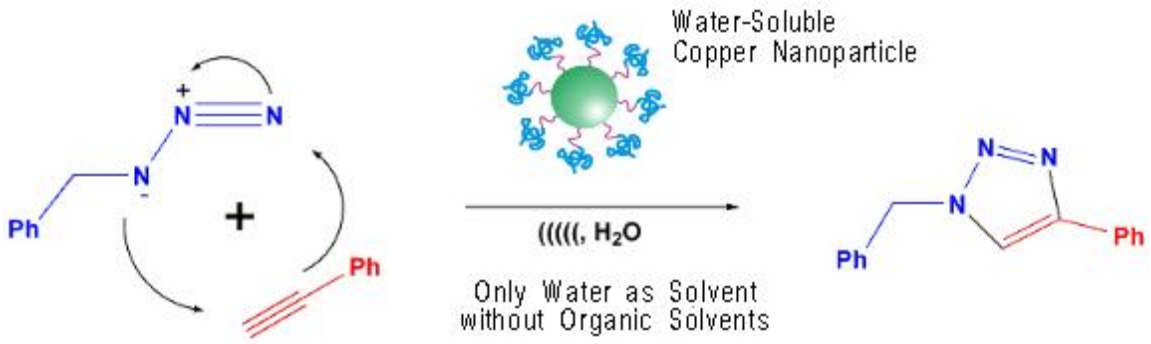
Alkyne-azide Click reaction catalyzed by water souble Copper Nanoparticles

김아람, 이현주, *김병수, 박강현

*부산대 화학과 *울산과학기술대 친환경에너지공학부*

A stable, water-soluble copper nanoparticle was synthesized using a double hydrophilic block copolymer as a template. The prepared nanoparticles were effective as a catalyst for the [3+2] cycloaddition of azides with terminal alkynes to provide products in good yields with high regioselectivity. An environmentally friendly process of synthesizing regioselective triazoles has been developed from a variety of azides with terminal alkynes, in which the water soluble copper nanoparticle is utilized, within ten minute under sonicating. The copper nanoparticles could be reused three times under the present reaction conditions without any loss of catalytic activity. We anticipate that the block copolymer nanoreactors are promising in creating a number of water-soluble catalytic metal nanoparticles for a wide variety of organic transformations.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

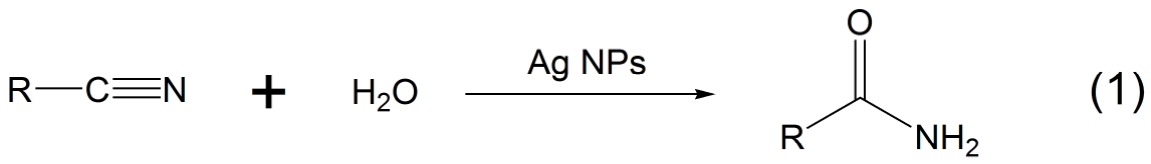
Silver Nanoparticles as Catalyst for Hydration of various nitriles

김아영, 배희선, *유찬용, 박강현

*부산대 화학과 *(주)제이피에스마이크로텍 기술연구소*

Hydration of nitriles into corresponding amide is very important to organic syntheses because amide can easily become a synthetic intermediate that is used for the production of pharmacological products, drug stabilizer, raw materials for engineering plastics, detergent, polymer, and lubricant. However, the traditional catalyst system needs an organic solvent in the presence of homogeneous strong acid and base catalysis.The big weaknesses of this classical method are: 1) harsh conditions that interfere with the existence of sensitive functional groups are generally required; and 2) it is difficult that a reaction stops at amide, and further, hydrolysis to the carboxylic acid often happens. In addition, in terms of industry, the last neutralization step causes unnecessary product contamination and makes huge salt (pollution effect). Therefore, chemists have strived for the development of the effective metal catalyst for the hydration of nitriles.

This paper reveals that Ag NPs can efficiently catalyze hydration of nitriles to amide in water. (Eq. (1)) This hydration method used water as a solvent and Ag catalyst that can be recycled under neutral conditions, so it can make a great contribution to settling the process that is environmentally better and industrially more satisfactory.



(1)

R = Alkyl, Aryl, Vinyl

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New Imido Tantalum Complexes: Potential Precursors for Atomic Layer Deposition

민재기, 박보근, 김창균, 정택모

한국화학연구원 화학소재연구단

Tantalum nitride (TaNx) films have been an attractive candidate as a diffusion barrier for copper-interconnect technologies because of their high thermal, mechanical, chemical stability, and good electrical conductivity. TaCN films (TaCN) also much interest as a metal gate electrode for its low film resistivity and thermal stability.Herein we report the syntheses and characterization of New imido based tantalum complexes.

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Synthesis and Structural Studies of Mn(II), Co(II/III), Ni(II), and Cu(II) Complexes with Schiff Base Derived from 2-Acetylpyridine

구본권

대구가톨릭대 화학과

Schiff bases containing *N*, *S* donor atoms and their metal complexes have received considerable attention owing to their potent biological activity as anti-fungals, anti-virals, anti-malarials, and most notably, as anti-tumour agents. In this work the complexes of Mn(II), Ni(II), Co(II/III), and Cu(II) of Schiff bases, acpy-mdtcH and acpy-phTscH, derived from 2-acetylpyridine and S-methyldithiocarbazate or 4-phenylthiosemicarbazone have been synthesized and characterized by elemental analysis, infrared spectroscopy, thermo gravimetric analysis, and single crystal X-ray diffraction. For an example, the reaction of $Ni(ClO_4)_2 \cdot 6H_2O$ with acpy-mdtcH yilded $[Ni_2(acpy\text{-}mdtc)_3]ClO_4 \cdot CH_3OH$. The X-ray structural analysis showed that the complex has a distorted six- and four-coordinated geometry with $Ni1N_4S_2$and $Ni2N_2S_2$chromophore, respectively.

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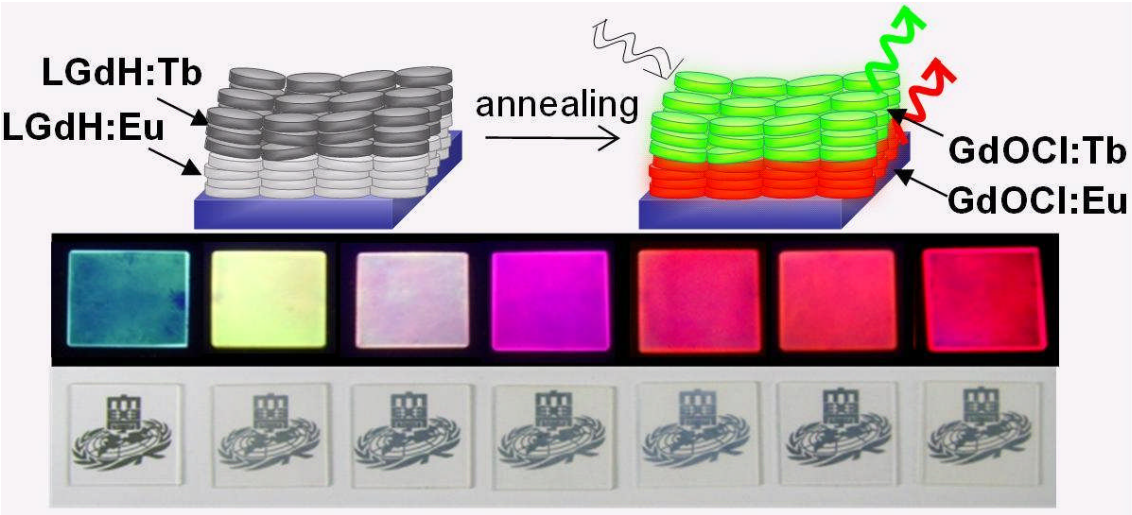
Unexplored Thermal Transformation Behavior of Two-Dimensionally Bound Gadolinium Hydroxide Layers:Fabrication of Oriented Crystalline Films of Gadolinium Oxychloride Nanosheets Suitable for the Multicolor Luminescence with Color Tunability

윤영수, 이인수

경희대 응용화학과

In this presentation, we would like to report the unexplored growth of well-oriented GdOCl crystallites from a layered gadolinium hydroxide multilayer with high two-dimensional anisotropy during a thermal annealing process via a spatially confined transformation mechanism. These findings were used to create a multilayer film composed of mixed GdOCl crystallites each doped with different activator ions, such as Eu3+ and Tb3+, which demonstrates a novel method of fabricating robust and semi-transparent inorganic thin films with multicolor emission capacity. We also demonstrate the possibility of modulating the luminescent color of the annealed film simply by adjusting the layer composition in reactant multilayer and combining discrete spectra from each activators.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

Stepwise Synthesis of Charged and Neutral Two-Dimensional Networks via One-Dimensional Silver(I) Coordination Polymer Based on Bis(4-pyridylmethyl)sulfide

박기민, 이심성

경상대 화학과

Stepwise synthesis and structural characterization of two-dimensional (2-D) coordination polymer frameworks with positive charged or neutral cavities are reported. First, reactions of bis(4-pyridylmethyl)sulfide (L) with silver salts (1: nitrate and 2: perchlorate) afforded the respective double-stranded one-dimensional (1-D) chains $[Ag(L)NO_3]_n$ (1) and $\{[Ag_2(L)_2](ClO_4)_2\}_n$ (2), both of which are stabilized by face-to-face π-π interactions. The difference of both structures indicates that the coordination ability of the anions has important effects on the silver(I) coordination environments. Interestingly, the perchlorato 1-D complex 2 allows further reactions with bridging ligands such as 4,4'-bipyridine (bpy) and terephthalate (tp^{2-}) to give a 2-D positive-charged network $\{[Ag_2(L)_2(bpy)]^{\cdot}(ClO_4)_2^{\cdot}3C_6H_6\}_n$ (3) and a 2-D neutral network $\{[Ag_2(L)_2(tp)]^{\cdot}2DMSO^{\cdot}6H_2O\}_n$ (4), respectively. The nitrato 1-D complex 1, however, showed no reactivity with the bridging ligands in the same condition. The results show that the replacement of anion by the bridging ligand in the coordination sphere of the 1-D precursor plays crucial roles in determining the reactivity for the synthesis of higher dimensional open frameworks.

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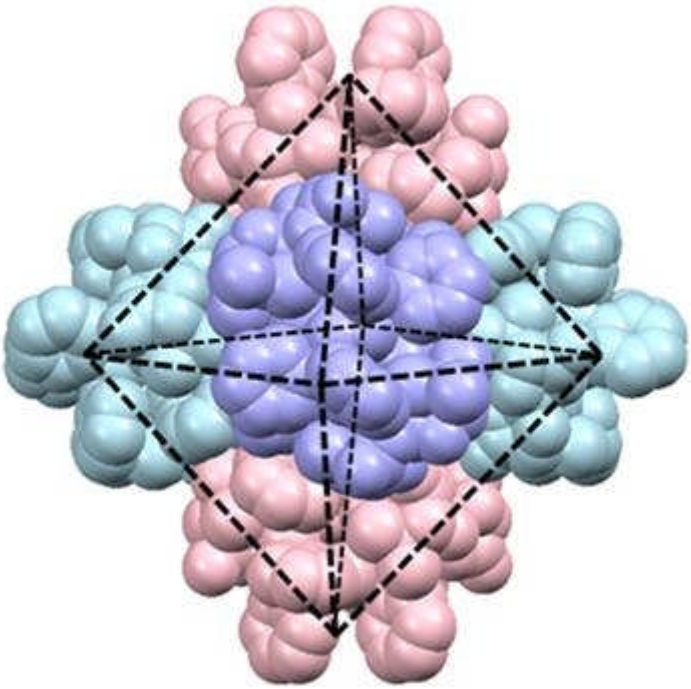
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Reactivity of a Diphosphine-Bridged Digold(I) Complex with D-Penicillaminate

Raeeun Lee, Asako Igashira-Kamiyama, Takumi Konno

Osaka University, Japan

Recently, we have shown that $[Au(D\text{-}pen)_2]^{3-}$ (D-H_2pen = D-Penicillamine) acts as a multidentate metalloligand to form a variety of multinuclear complexes. To extend this metalloligand system, we though it worthwhile to replace an Au^I ion in $[Au(D\text{-}pen)_2]^{3-}$ by a diphosphine-digold(I) unit that provides flexibility and structural diversity to the system. Here we report on the preparation of $[Au_2(D\text{-}Hpen)_2(dppe)]$ (dppe = bis(diphenylphosphino)ethane), in which two [Au(D-Hpen)] units are linked by a dppe ligand. The reaction of this digold(I) complex with Co^{III}, which leads to the formation of a fascinating supramolecular structure, will also be reported



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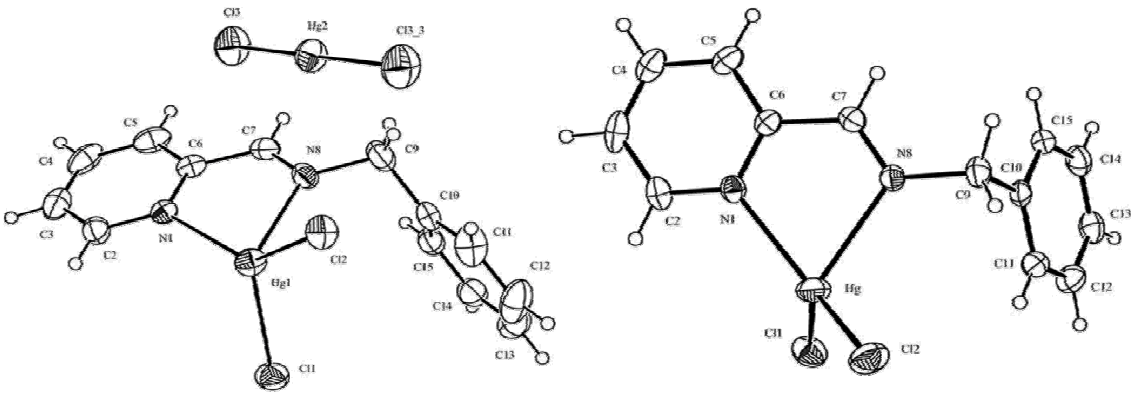
발표종류: 포스터, 발표일시: 목 15:00~17:00

Hg(II) Complexes with Schiff-base Derived from Benzylamine and 2-Pyridinecarboxaldehyde: Crystal Structure and Luminescent Properties

윤성재, 서희주, *송영광, 김인찬, **김영인

*부산대 화학과 *부산대 첨단정보 및 디스플레이소재협동과정 **부산대 화학교육과*

Schiff-base ligand of (E)-1-phenyl-N-(pyridin-2-ylmethylene)methanamine (ppmma) and its $HgCl_2$ complex with the formula of (ppmma) $HgCl_2$ was synthesized. The ppmma ligand coordinated to Hg(II) ions in bidentate mode showing bright blue emission and exhibited two type crystal structures: (ppmma)$HgCl_2$ (white) and $[(ppmma)HgCl_2]_2 \cdot HgCl_2$ (yellow) The photoluminescence showed that the emission of Hg(II) complex was blue-shift than that of ppmma ligand and the quantum yield was increased in Hg(II) complex. The emission was contributed from the intra ligand (IL) π- π^* transition. The role of Hg(II) metal ion in the complexes stabilized the ligand via the formation of coordination bonds.



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Synthesis of $CuInSe_2$ Nanocrystals in Aqueous Media and Their characterization

Jin Xing, 김진권

공주대 화학과

$CuInSe_2$ is a I–III–VI_2 semiconductor compound with properties suitable for photovoltaic applications. Laboratory-scale solar cells using this compound reached efficiency values of up to 17%. $CuInSe_2$ is considered as a potential material for thin-film solar cells because its high optical absorption coefficient, high stability and low band gap. Herein we present an aqueous phase synthetic route for $CuInSe_2$ nanoparticles. In our synthesis, the Se precursor used was Na_2SeSO_3 and CuI and $InCl_3$ were used as precursors for copper and Indium, respectively. The reaction was performed in water under basic condition and thioglycolic acid (TGA) also was used during the reaction. It was concluded form our results that TGA effectively stabilized metal ions in aqueous media. The reaction ratio of each component was optimized and the nanocrystals obtained were characterized by XRD, SEM, TEM, XPS, TG/DSC.

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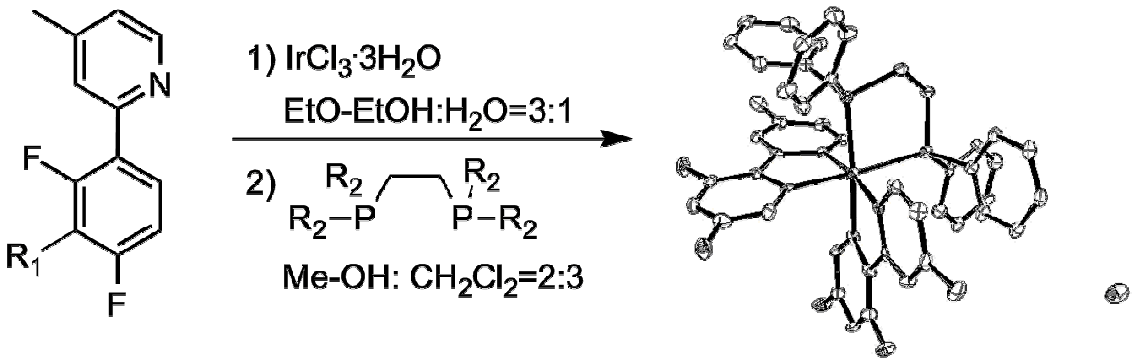
발표종류: 포스터, 발표일시: 목 15:00~17:00

Deep-Blue Emitting Cationic Iridium Complexes with Diphophine Ligands for Highly Efficient Organic Light-Emitting Diodes

서희주, 윤성재, *송영광, 김인찬, **진성호, **김영인

*부산대 화학과 *부산대 첨단정보 및 디스플레이소재협동과정 **부산대 화학교육과*

New cationic iridium(III) complexes containg two phenylpyridine-based ligands and one diphosphine as bidentate ancillary ligand were prepared : $(dfpmpy)_2Ir(dmpe)$ (1), $(dfpmpy)_2Ir(dppe)$ (2) $(dfpmpyCF_3)_2Ir(dmpe)$ (3) and $(dfpmpyCF_3)_2Ir(dppe)$ (4), where dfpmpy=2-(2',4'-difluorophenyl)-4-methylpyridine, $dfpmpyCF_3$=2-(2',4'-difluoro-3'-trifluoromethylphenyl)-4-methylpyridine, dmpe=1,2-bis(dimethylphosphino)ethane and dppe=1,2-bis(diphenylphosphino)ethane. The structural and photophysical properties were investigated. The complexes 3 showed deep-blue emission of 436 nm and high quantum yield of 45%. The fabricated OLEDs showed high external quantum efficiency (1.42%) and current efficiency (2.35cd/A) with the CIE coordinate for (0.14, 0.27).



L1 R_1 = H

L2 R_1 = CF_3

1 R_1 = H, R_2 = CH_3

2 R_1 = H, R_2 = phenyl

3 R_1 = CF_3, R_2 = CH_3

4 R_1 = CF_3, R_2 = phenyl

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Strong Blue Luminescent Copper(I) Coordination Polymers: Luminescence Vapochromism by I^{-}•••H—O Hydrogen Bond

양호진, 김태호, 박가람, 김진은

경상대 화학과

Recently, there has been considerable interest in phosphorescent transition metal complexes because of their potential applications in flat-panel displays and lighting sources. We have explored coordination polymers based on dithioether ligands and $(CuI)_x$. As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we introduced an aromatic nitrogen donor instead of a sulfur donor. There are some reports on Cu(I) complexes with N/P mixed donor ligands, N/S mixed donor ligands are still scant. Our investigation focuses on new $(CuI)_x$ coordination polymers ($x=2,3,\infty$) based on an N/S mixed donor ligand, 4-(3-pyridinylcarbonyl)-thiomorpholine. The results of our investigation including syntheses, structural characterization, thermal and luminescent vapochromism properties of four new Cu(I) coordination polymers are presented. In addition, preparation of four coordination polymers 1-4 from a luminescent nanosphere intermediate will be exhibited.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Luminescent Cu(I) Coordination Polymers Based on N, S Donor Ligand

김현지, 박가람, 양호진, 김태호, 김진은

경상대 화학과

Recently, we have explored coordination polymers based on dithioether ligands and $(CuI)_x$. As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we synthesized a N,S donor ligand, *N*-(3-pyridylmethyl)-2-(cyclohexylthio)acetamide, (L^1) and *N*-(3-pyridylmethyl)-2-(benzylthio)acetamide, (L^2). And, two Cu(I) coordination polymers 1 and 2 based on the ligands were prepared. Polymers 1 and 2 are composed of rhomboidal Cu_2I_2 nodes, emitting blue light. The results of our investigation including syntheses, structural characterization, thermal and photoluminescent properties of two new Cu(I) coordination polymers are presented.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Nanoporous $ZnO/Zn(OH)_2$ Sphere and Its Replication to High Surface TiO_2 Materials

허성, 황용경

한국외국어대 화학과

Highly crystalline mesoporous $ZnO/Zn(OH)_2$ spheres with decent surface area were prepared by a simple single-step method. The spheres were fully characterized by photoluminescence study, gas sorption analysis, and electron microscopy. The hydrolytically unstable nature of the $ZnO/Zn(OH)_2$ composite makes it an ideal hard template for other metal oxides. For example, amorphous TiO_2 (TiO_2-300-3) with high surface area of 525 m^2 g^{-1} was obtained after an acid-etching of the $ZnO/Zn(OH)_2$ template from the $TiO_2/ZnO/Zn(OH)_2$ hybrid material. This amorphous TiO_2 material could be crystallized into anatase-rich phase with surface area up to 202 m^2 g^{-1} for TiO_2-350-24. TiO_2-350-24 is a good photocatalyst for the decomposition of methyl orange under UV irradiation. Currently, we are exploiting preparations of other catalytically active metal oxides through $ZnO/Zn(OH)_2$ composite templating approach.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Soultion-Phase Synthesis of Anisotropic Au Materials:Use of Surfactants as Shape-Directing Agents

유효종

한림대 자연과학대학 화학과

We show the synthesis of anisotropic Au fibers with micron-scale lengths and Au rings via a solution-phase synthetic method. Solubilization of salicylate ion into an aqueous cetyltrimethylammonium bromide (CTAB) surfactant solution forms rod-shaped micelles and becomes a key shape directing factor to generate one-dimensional growth of Au structures. By use of a Au^{3+} precursor and commercially available nonionic surfactant ($(C_2H_4O)_{23}C_{12}H_{25}OH$, Brij®35), we could generate Au rings through a single-step, one-pot synthesis. We show the controllable growth of Au_{core}-Pd_{shell} nanostructures. The heteroepitaxial growth of Pd is dominated in high amount of CTAB, since the generation of Pd-CTAB complex can decrease the reduction rate, and the reaction can be controlled kinetically.

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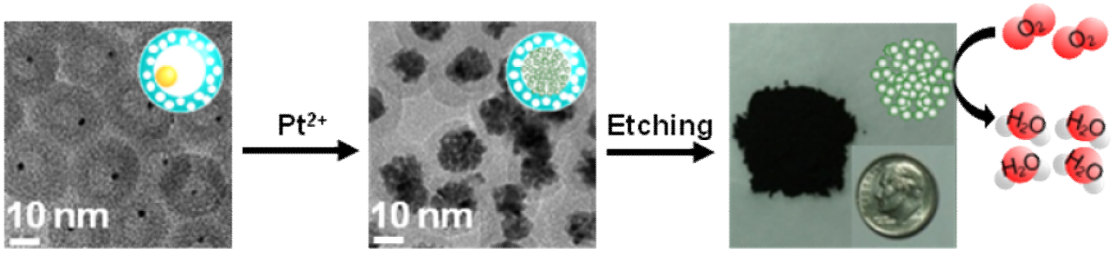
High-concentration Synthesis of Surfactant-Free Pt-on-Au Nanodendrites with Enhanced Catalytic Performance for Oxygen Reduction by Employing Seed Mediated Growth inside Porous Hollow Silica Nanosphere

여경민, *최수희, *김종원, 이인수

*경희대 응용화학과 *충북대 화학과*

This presentation reports the novel synthesis of Pt nanodendrites via Au-seed mediated growth inside hollow silica nanospheres. The synthetic protocol proposed in this study based on isolated nanoreactors is quite remarkable in terms of the product yield per unit reaction volume compared to traditional capping-agent based synthesis, which produces only a few mg of Pt nanodendrites per 1 ml of reaction suspension. The nanoreactor-based synthetic route enabled the synthesis of as much as 1.5 g of uniform Pt nanodendrites from a single reaction in a 40 ml aqueous suspension. The prepared ligand-free Pt nanodendrites exhibited greater ORR activity than commercial Pt black catalysts. We also demonstrate the extendable utility of the current method to prepare Pt nanodendrites colloid with tunable dispersity and hybrid nanocrystals of various novel metals.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of $AlPO_4$-type Mesoporous Materials from Alum Sludge

강광철, *강미선, *이석우

*공주대 그린홈에너지기술연구소 *공주대 화학과*

In this study, a novel AlPO4-type porous materials were synthesized by the reaction of aluminum hydroxide and phosphoric acid with organic templates. Cationic surfactant, natural humic acid, and amino acids were used for organic template. Powder X-ray diffraction patterns showed that the materials were well-defined AlPO4-type materials. The change of surface morphology of the materials was examined using scanning electron microscopy. The specific surface area and pore size distribution of the material were analyzed by BET measurement. In conclusion, the template-assisted synthetic method provided AlPO4-type porous materials which might be applicable in removal of toxic formaldehyde in the air.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation and structure supramolecular complexes combined tetraaza complexes and cyanoargentates

김성민

순천대 화학전공

Cyano-argentates ($[Ag_x(CN)_y]^{x-y}$) are elegant building blocks for molecular tectonics because they have a variety of coordination or assembly pattern with cationic counter parts. Thus, they are viable design tectons which can be used to increase dimensionality and influence the supramolecular structures. Furthermore, argentophilicity will help increase of the dimensionality of resulting supramolecule. We performed the preparation of combined tetraaza macrocyclic complexes with $[Ag(CN)_2]^-$ to explore the network pattern of these in crystal. Here we present preparation and characterization of the obtained supramolecules.

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Synthesis and Characterization of N,N'-Dibenzyl-(R,R)-1,2-Diaminocyclohexanes with o- or p- fluoro Substituents Dichloro Cu(II) and Its Catalytic Application in Asymmetric Henry Reaction

정연희, 정종화

경북대 화학과

The availability of newer types of chiral catalysts coupled with the ever-increasing requirements for stereochemically pure amino alcohols in pharmaceutical and natural product synthesis has made the evolution of the Henry reaction possible. We synthesized the Cu(II) complexes of N,N'-Dibenzyl-(R,R)-1,2-Diaminocyclohexanes with o- or p- fluoro Substituents. The X-ray crystallography of N,N'-bis-p-fluorobenzyl-(R,R)-1,2-diaminocyclohexane with Cu(II) was studied. X-ray structure data shows that geometry around the central Cu(II) metal is distorted square planar. The coordination of the metal to the chiral amine ligand leads to a 5-membered heterocyclic ring that blocks nitrogens in (S,S)-configuration. Asymmetric nitroaldol reaction between benzaldehyde and nitromethane in the presence of diisopropylethylamine and the chiral complexes as enantioselective catalysts was examined.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Zn(II) and Cu(II) Complexes Bearing [N,N'-Bis(4-Methoxybenzyl)-(R,R)-1,2-Diaminocyclohexane] ligand and Catalytic Asymmetric Henry Reaction of Benzaldehyde

정연희, 정종화

경북대 화학과

New chiral Zn(II) and Cu(II) complexes potentially useful for the asymmetric catalysis has been synthesized. The complexation reaction of N,N'-Bis(4-Methoxybenzyl)-(R,R)-1,2-Diaminocyclohexane(L1) with ZnCl2 and CuCl2. X-ray crystal structures of these complexes reveal that Zn complex in the geometry of distorted tetrahedral fashion, but the Cu one in nearly square-planar. The coordination of metals to the chiral amine ligand leads to a 5-membered metallaheterocycle of (S,S) configuration. In both cases, the original C2-symmetry of the ligand was preserved. Their asymmetric catalytic activities for nitroaldol reaction of benzaldehyde were examined. Interestingly, the amine nitrogen of L1ZnCl2 complex was found to exhibit only (R) configuration while that of L1CuCl2 complex have(S) configuration.

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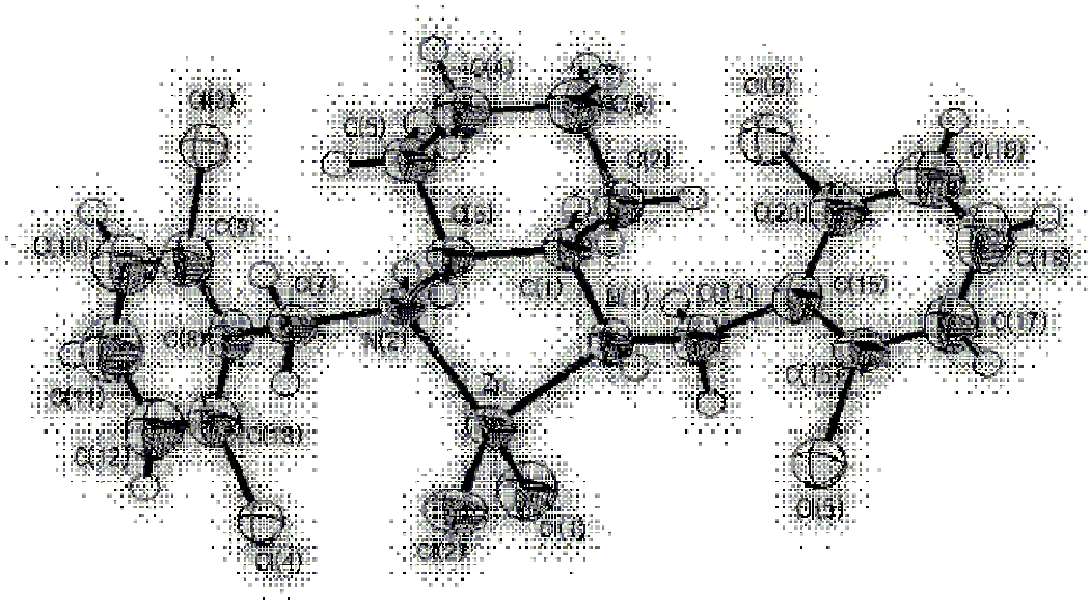
Ring Opening Polymerization of rac-Lactide Initiated by In-situ Zinc Dimethyl Complexes Derived from (R,R)-1,2-Cyclohexane diamine Ligand

Nayab Saira, *이효선, 정종화

*경북대 화학과 *경북대 자연과학대학 화학과*

New zinc complexes based on bidentate ligands (N,N'-Dibenzyl-1,2-cyclohexane diamine) and N,N'-Bis-(2,6-dichloro-benzyl)-1,2-cycloexane diamine have been synthesized in high yield and purity. The crystal structures of the complexes were determined by x-ray crystallography. The well characterized complexes were employed as an initiator for ring opening polymerization of rac-Lactide. The complexes were found to be highly efficient initiator yielding the PLA with well molecular control and narrow molecular weight distribution. Experimental results indicate that the catalytic activity of the complex [C6H8 {(NH)2(C6H5)2}ZnCl2] was dramatically affected by the electronic effect of substituent's on the cyclohexamine. Furthermore, the heterotactic PLA with Pr up to 80 % can be obtained by initiating ROP of rac-lactide in CH2Cl2 at -23℃. The molecular weight of the polymer was determined by GPC.



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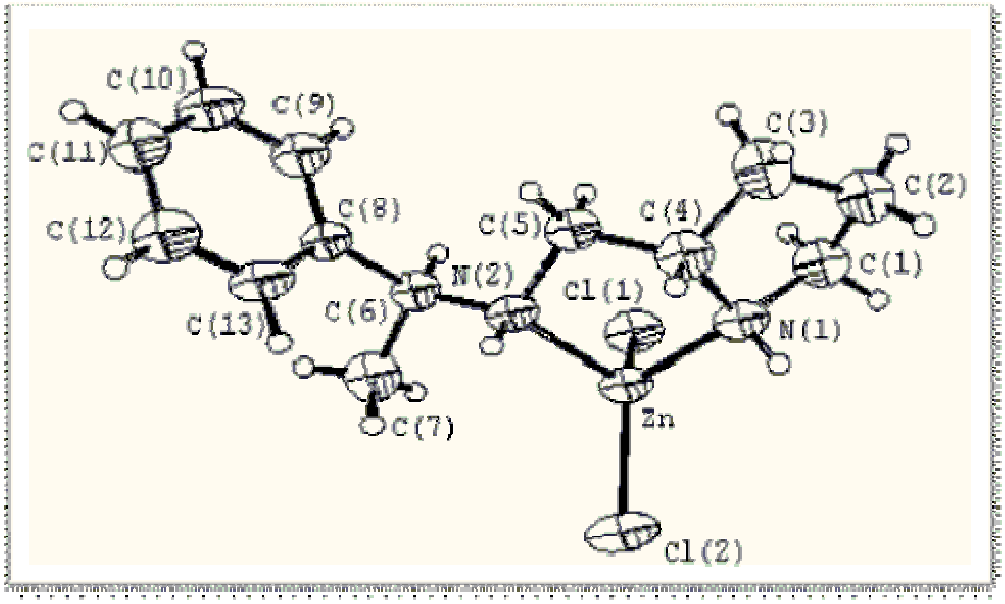
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and X-ray Crystal Structure of Dichloro[(1-Phenyl-ethyl)-pyrrolidin-2-yl methyl-amine] Zinc (II) and Its Catalytic Application to rac-Lactide Polymerization

Nayab Saira, *이효선, 정종화

*경북대 화학과 *경북대 자연과학대학 화학과*

The biocompatible nature of polylactide (PLA) has promoted the use of biocompatible metals because trace amount of the catalyst may be tenaciously incorporated within the polymer. New zinc dichloro complex ligated by the homochiral chiral bidentate ligand [(1-Phenyl-ethyl)-pyrrolidin-2-yl methyl-amine] has been synthesized in high yield and purity. The synthesized complex is characterized by various spectroscopic techniques. The crystal structure of the complex was determined by x-ray crystallography and its catalytic capacity was evaluated in Ring Opening Polymerization (ROP) of rac-Lactide. The active catalyst species was generated by treating air and moisture stable ZnCl2 complex with MeLi in situ. The metal complex was found to be highly active for ROP of rac-lactide and give preference to heterotactic polylactide. The thermal behavior and molecular weight of the obtained polymer was determined by DSC, and GPC, respectively.



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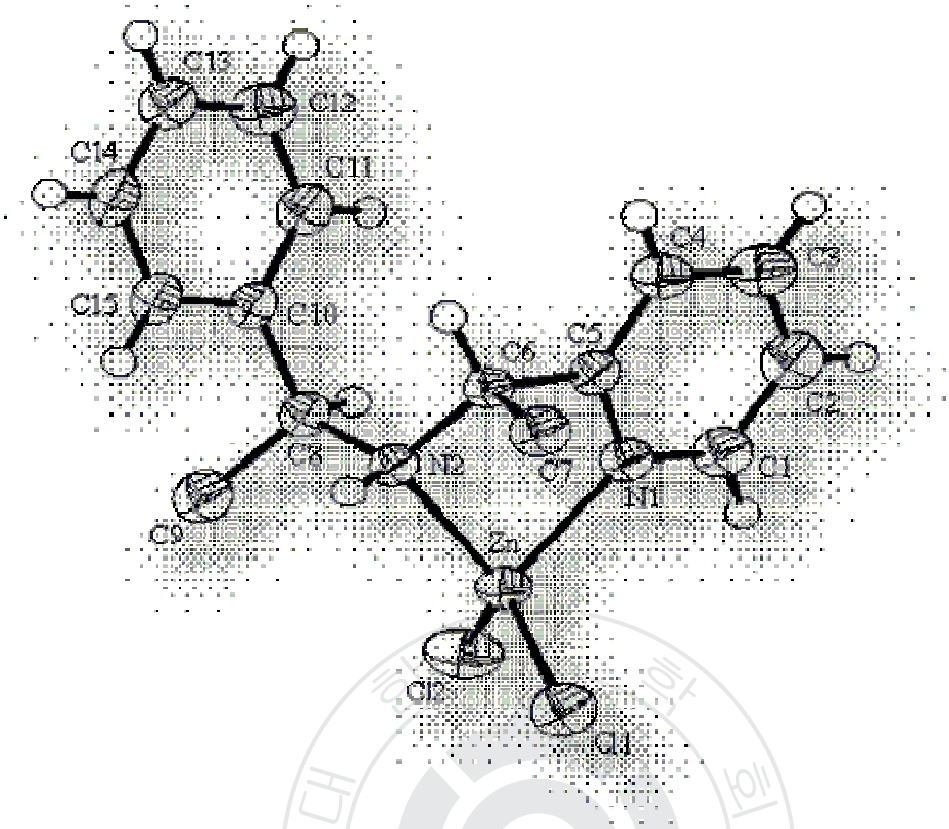
발표종류: 포스터, 발표일시: 목 15:00~17:00

Zinc Complexes Based on Bidentate Homochiral Nitrogen Ligands: Synthesis, Structures, and Catalytic Activities to Ring Opening Polymerization o f rac-Lactide

Nayab Saira, *이효선, 정종화

*경북대 화학과 *경북대 자연과학대학 화학과*

Polylactide is one of the most important biodegradable polymers due to their biomedical and pharmaceutical applications. ROP of lactide using non hazardous zinc complexes has attracted great attention than highly toxic tin and lead.The attempt was carried out to prepare the PLA with the newly synthesized zinc complexes based on bidentate (1-Phenyl-ethyl)-(1-pyridin-2-yl-ethyl)-amine and (1-Phenyl-ethyl)-pyridin-2-ylmethyl-amine ligands. The synthesized complexes are characterized by various spectroscopic techniques in addition to x-ray crystallographic structure determination. The well characterized complexes were evaluated for the ring opening polymerization of rac-Lactide. Zinc complexes supported by homochiral ligands showed high activity for rac-Lactide and heterotactic selectivity. The heterotactic PLA with Pr up to 88 % can be obtained by initiating ROP of rac-lactide in CH2Cl2 at -23℃. Furthermore, the molecular weight and polydispersities of the obtained polymer was determined by GPC.



대 한 화 학 회
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일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Syntheses and Characterization of Fe, Ni, Ru Complexes Containing N,N'-(ethylenedi-*p*-phenylene)bis(pyridine-2-carboxamide) Ligand

김동훈, shuranjan sarkar, 이홍인

경북대 화학과

The carboxamide group, found in the primary structure of proteins, is an important ligand construction unit for coordination chemistry. Phenyl-pyridyl-carboxamides, a growing class of multidentate ligands containing this linkage, are available from condensation reactions between pyridyl-bearing carboxylic acids and phenyl amine precursors, promoted by coupling agents such as triphenylphosphite. The deprotonated carboxamide nitrogen atom and the pyridyl ring chelate metal ions. These types of metal complexes have been found useful in asymmetric catalysis, molecular receptors and dendrimer synthesis. We are interested in the catalytic behaviors of these types of metal complexes for selective organic transformation. We have synthesized and characterized the iron, nickel, and ruthenium complexes with N,N'-(ethylenedi-*p*-phenylene)bis(pyridine-2-carboxamide)(H_2L) by elementalanalysis, FABmass, IR and UV-vis spectroscopy, respectively.

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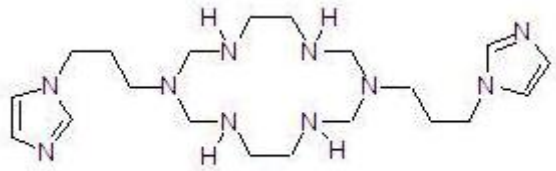
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Structures and Properties of Ni(II) Hexaazamacrocycles Containing Bridging Ligands

김태형, 김주창

부경대 화학과

Coordination polymers $[Ni(L)(BL)]_n$ (1) (where L = 1,8-di(1-propyl-imidazole)-1,3,6,8,10,13-hexaazacyclotetradecane, BL = Bridging Ligands) have been synthesized and structurally characterized by a combination of analytical, spectroscopic and X-ray diffraction methods. The basic structural feature of each complex shows a 1D chain, where nickel (II) ions are connected with bridging ligands. The complexes were prepared by the reaction between $[Ni(L)](HClO_4)_2(ClO_4)_2$ and appropriate bridging ligands. The details of the structures and spectroscopic properties were described in this presentation.



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장소: 대구엑스코
발표코드: **INOR.P-74**
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발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of Novel Strontium β-diketiminate Complex

조지쉐비메리, 박보근, *연규환, 김창균, 정택모

*한국화학연구원 화학소재연구단 *한국화학연구원 화학물질연구단*

Organometallic chemistry of heavier alkaline earth metals, strontium and barium, have attracted interests due to their applications in organic synthesis and polymerization as well as in thin film chemistry as precursors. The chemical vapor deposition (CVD) and atomic layer deposition (ALD) method require high volatile precursors for efficient vapor transport. In addition, ALD precursors must be thermally stable at film growth temperatures. The β-diketiminate ligand will give stable complex with stronitum due to their mono anionic nature, the chelating capacity with variable mode of hapticity. A new β-diketiminate complex of strontium was synthesized by treating LH (β-diketiminate ligand) with strontium(btsa)2 to yield SrL2 . The SrL_2 was crystallized in monoclinic space group from the hexane solution upon cooling. The compound was characterized using NMR spectroscopy and Elemental Analysis. The crystals grown from the parent solution were studied by single crystal X-ray diffractometer which reveals that SrL2 crystallized in monoclinic space group. The thermo gravimetric analysis of SrL2 was carried out to measure the decomposition character and volatility of the complex.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Microporous Metal-Organic Frameworks: High Gas Sorption Properties and Metal Ion Exchange

홍대호, 백명현

서울대 화학부

3D metal-organic frameworks, 1 and 2, have been prepared by the solvothermal reactions of tetracarboxylate ligand with Cu and Zn, respectively. Framework 1 has an NbO type net structure while 2 has a PtS type net structure. Desolvated 1 adsorbs high amounts of N_2, H_2, O_2, CO_2, and CH_4 gases due to the presence of a vacant coordination site at every metal ion as well as the imide groups in the ligand. By the metal ion exchange of 2 with Cu, PtS type net was prepared, which could not be synthesized from the direct solvothermal reaction.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of New Antimony(III) Complexes with Donor-functionalized Ligands for CVD and ALD Precursors

정인경, 김창균, 정택모, 박보근

한국화학연구원 화학소재연구단

Antimony(III) complexes with donor-functionalized ligands have been proposed as potential CVD precursors to thin films of bismuth-containing materials. The virtual absence of antimony complexes stabilized by chelating ligands is surprising, since chelating frameworks may potentially be used in tailoring the thermal, photolytic, and hydrolytic stability of these compounds. Antimony complexes are currently attracting great interest because of its myriad applications in organic and oxidation catalysis, medicine and biochemistry, superconductors, ferroelectrics, and many other oxide based materials. Particularly, antimony compounds have application to phase changing $Ge_2Sb_2Te_5$ (GST) thin films. Phase changing $Ge_2Sb_2Te_5$ (GST) thin films has attracted considerable attention from the semiconductor memory field considering its key role in the fabrication of highly integrated phase change random access memory devices (PcRAM).New compounds have been characterized by NMR, FT-IR and elemental analysis. Thermal analysis has also been performed to qualitatively evaluate their volatility and thermal stability for potential use as CVD and ALD precursors.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Superconductivity of Niobium Nitride Nanoparticles within a Mesoporous Core/Shell Silica Microsphere

한승현, 이종인, 유정보, 김미현, 강승희, 이규형, 허남회

서강대 화학과

We report the synthesis and characterization of niobium nitride nanoparticles embedded in mesoporous shells of a core/shell silica microsphere (NbN@SiO2). Using two immiscible solvents, niobium precursors were incorporated into mesoporous shells, followed by annealing at high temperature under the ammonia atmosphere. The resulting NbN@SiO2 microspheres were characterized by powder X-ray Diffraction, TEM, EDX, XPS, and magnetization measurements using a SQUID magnetometer. The niobium nitride nanoparticles show a superconducting transition at 8 K and unusual field-dependent magnetization property. We discuss the superconducting properties of NbN@SiO2 by comparison with those of bulk NbN powders.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Syntheses and Crystal Structures of Metal (Mn, Co) Organic Frameworks Constructed by Using Tricarboxylate Ligands

심수연, 조장훈, *나명수, **이하진, 이홍인

*경북대 화학과 *울산과학기술대 친환경에너지공학부 **한국기초과학지원연구원 전주센터*

We obtained three new metal organic frameworks (MOFs) from the reactions between Mn(Ⅱ) and 1,3,5-cyclohexanetricarboxylic acid (1,3,5-CTC), Co(Ⅱ) and 1,3,5-CTC, and Mn(Ⅱ) and 1,3,5-benzenetricarboxylic acid (1,3,5-BTC). X-ray crystallographic studies revealed that all three compounds have linear tri-nuclear metal centers working as a node. Six carboxylate ligands coordinated to each center and the nodes are connected through the ligands to form 2D-network structure for the Co compound and 3D-network structure for the Mn compounds. The metal-metal distances were found to be 3.11 - 3.93 Å. In this poster, we describe the crystal structures, the thermal stability, and other properties.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

A microporous 3D metal-organic framework having an eight-connected pentanuclear secondary building unit

정석, *정세현, *Song xiaokai, **나명수

*울산과학기술대 친환경에너지공학과 *한양대 응용화학과 **울산과학기술대 친환경에너지공학부*

A metal-organic framework (MOF), $[(Mn^{II}_5O_2)L_4S_8]$ (1), was prepared using a new ligand, 2,6-di(1H-tetrazol-5-yl)naphthalene (2,6-H_2NDT), in which two tetrazole units are connected via the naphthalene group. The single crystal diffraction study reveals that 1 is constructed from pentanuclear $\{Mn^{II}_5\}$ building-blocks and the ligand in $HNDT^{-1}$ and NDT^{2-}protonation states. The ligands in $HNDT^{-1}/NDT^{2-}$ protonation states offer a very rich coordination chemistry as a result of having two tetrazolate rings, each with three/four possible donor nitrogen atoms and may supply diverse coordination modes. It shows that the tetrazolate groups adopt a monodentate binding mode, bidentate (1,2-μ and 2,3-μ bridging) binding modes, and a tridentate binding mode with the Mn^{II} centers in 1. In pentanuclear $\{Mn^{II}_5\}$ building-block, there are three unique Mn atoms and one of them is on the inversion center. All the three unique Mn atoms are in an octahedron environment and bridged via a μ^3-oxo anion to each other. Each pentanuclear unit is connected to eight neighboring clusters, which can be considered an eight-connected node, to form the 3D MOF, 1. It possesses a narrow 1D solvent channel, which comprises about 30.0% of the whole crystal volume after removing the lattice solvent molecules.

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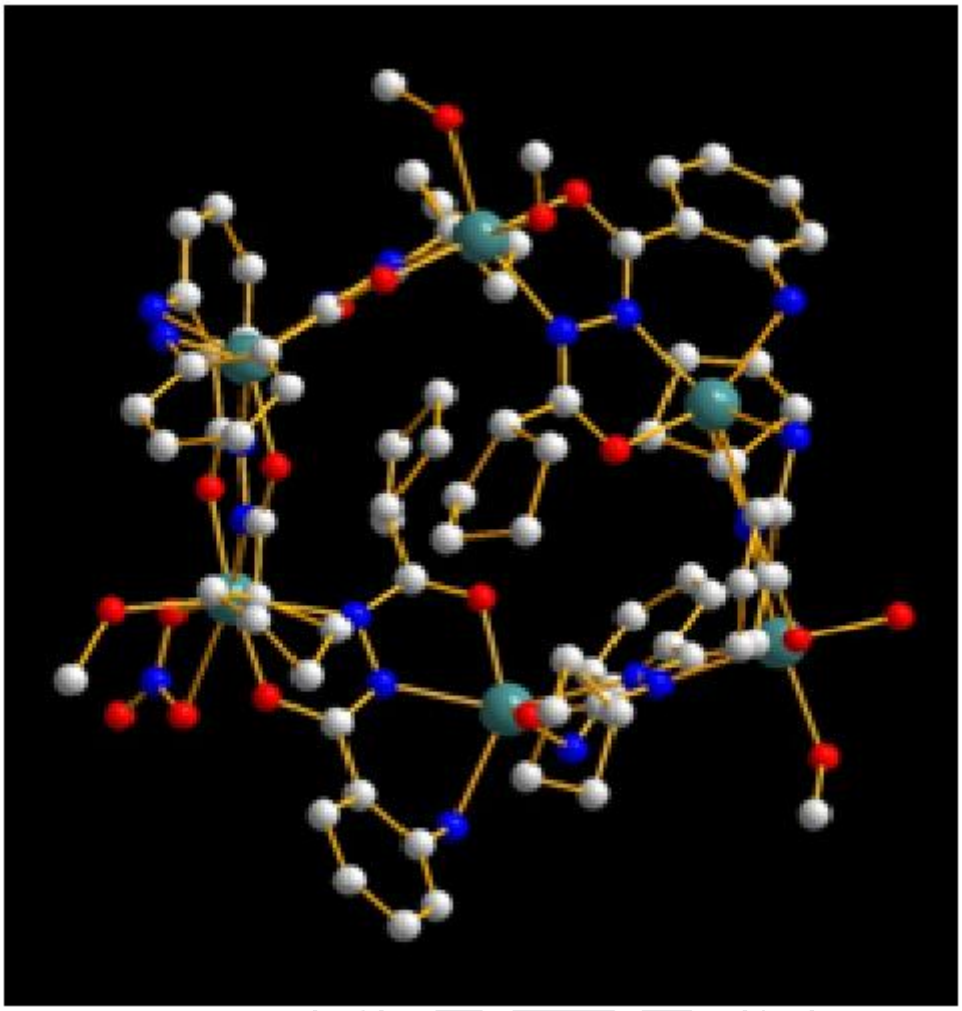
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Hexanuclear Indium Metal-Organic Macrocycles with Large Ring Strain

오민학, Liu Xinfang, 김동욱, *나명수

*한양대 응용화학과 *울산과학기술대 친환경에너지공학부*

An 18-membered hexanuclear metal-organic macrocycle (MOM), $[In(III)_6(H_2L^4)_6(NO_3)S_5](NO_3)_5$, (S is either methanol or water molecule), 1, has been synthesized using a pentadentate ligand N-cyclopentanoylaminobenzoylhydrazide (H_2L^4) with indium nitrate hydrate. Two different types of the coordination geometry of the indium centers were observed in 1. One is in a mer-tridentate/tridentate chelation mode and the other is in a cis-bidentate/bidentate chelation mode. A repeat of the two alternating chiral metal centers leads to the pseudo D_3-symmetry hexanuclear In-MOM, where the metal centers are in the •••$(M_cM_\Delta)(M_cM_\Delta)$••• chiral sequence. As in the D_4-symmetry Ga-MOM with alternating two different chiral metal centers, there are two different types of M•••M•••M angles in 1. The formation of an In-MOM with smaller ring size is unfavorable enthalpically because of the increased ring strain. However, the combination of the larger tolerance toward the more distorted coordination geometry of the metal centers having soft coordination characteristic and a small enthalpic cost for the ligand deformation from the conjugated planar conformation allows the formation of the D_3-symmetry hexanuclear 18-membered In-MOM. The detailed features of the indium macrocycle will be discussed.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation and Properties of supramolecules of Tetraaza Complexes of Nickel(II) and Copper(II) cooperating with [Fe(CN)6]3- Building Block

엔크줄

순천대 화학과

[Fe(CN)6]3- has been revealed as an useful building block to produce cyanide bridged networks with a various type of cationic complexes. Some network systems show distinctive photochemical and magnetic properties, or characteristic molecular sieve derived from the multidimensional structure and electronic property. We prepared two different multimetallic systems of Cu(II) and Ni(II) complexes of tetraazamacrocycle(L) incooperated by [Fe(CN)6]3-. In this presentation, preparation and properties of [NiL]3[Fe(CN)6]2 and [CuL]([CuL] [Fe(CN)6])2, (L=3,10-dihydroxyethyl-1,3,6,8,10,12-hexaazacyclotetradecane) will be discussed along with the X-ray structure of them.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Fluorescent Chemosensor for Carbonyl group

주리라

이화여대 화학나노과학과

Recognition and sensing of anionic substrates by neutral or positively charged synthetic receptors have attracted much attention because of the fundamental roles of anions in many chemical and biological processes. The copper complex was applied on recognition of a series of anions, fluorescence titration experiments revealed that it can selectively recognize pyridine from other anions by a significant fluorescence enhancement effect, whereas, other anions do not leading to obvious fluorescence changing. The binding of copper complex and pyridine was proved to form 1:1 host-guest interaction by single crystal X-ray diffraction analysis.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation and structure of Cu(II) and Ni(II) complexes of tris(2-aminoethyl)amine with oxalate and carbona

엔크줄

순천대 화학과

The coordination chemistry of complexes derived from tris(2-minoethyl) amine (tren), a kind of tripodal ligand, is interesting because it implies wide variety of biochemical activities. Especially, it's multinuclear complexes is important because it can be an useful model to evaluate the role of multinuclear metalloenzyme. All title compounds contain the [M(tren)]2+ cation [tren=tris(2-aminoethyl)amine]. The tren molecule acts as a tetradentate ligand around the central metal ion. These complexes show that metal ions bridged by oxalato or carbonato ligand.The m-CO32- bridged Ni(II), Cu(II) complexes with tris(2-aminoethyl)amine (tren), [M3(tren)3(m-CO3)]4+ was obtained by the reaction of tren, Na2CO3 and nickel(II) or copper(II) ion in an aqueous solution. The dinuclear nickel(II) complex [Ni2(C2O4)(tren)2][ClO4]2 has been synthesized by same method except Na2C2O4 was used instead of Na2CO3 and characterized by single-crystal X-ray diffraction

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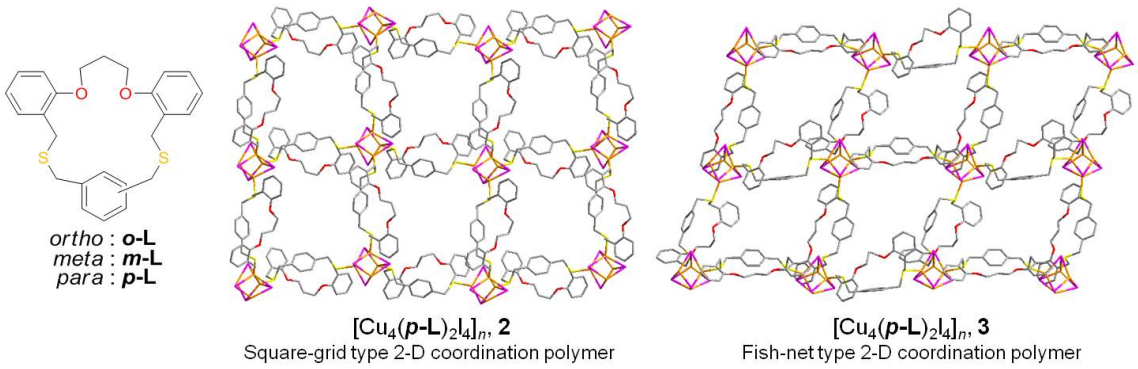
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Tribenzo-O_2S_2-Macrocyclic Isomers as Building Blocks for Coordination Polymers

김현지, *Leonard F. Lindoy, 이심성

*경상대 화학과 *School of Chemistry, The University of Sydney*

Tribenzo-O_2S_2-macrocyclic isomers incorporating a xylyl group in ortho (*o*-L), meta (*m*-L), and para (*p*-L) positions were employed to examine the effect of ligand isomers on supramolecular networking system. Self-assembly and photophysical properties of exo-coordination-based CuI coordination polymer of tribenzo-O_2S_2-macrocycles are reported. Reactions of CuI with *m*-L afforded mixed product with pale-yellow color block crystals 1a and powder 1b. 1a is a 2-D polymeric array of formula $[(Cu_2I_2)(m\text{-L})_2]_n$. In contrast to 1a, 1b exhibits a broad band with bright-yellow emission maxima at 570 nm arising from the cluster-centered excited state with mixed halide-to-metal charge transfer character. Meanwhile, reaction of copper(I) iodide with *p*-L afforded an emissive square-grid (2) and fish-net (3) type 2-D coordination polymers via Cu_4I_4 cubane core. On the other hand, in case of mercury(II) thiocyanate, *o*-L and *p*-L afforded infinite 1-D linear and zigzag coordination polymer networks, respectively. But *m*-L gave 2-D square grid type network. All three polymeric structures show different thiocyanate binding motifs.



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발표코드: **INOR.P-85**
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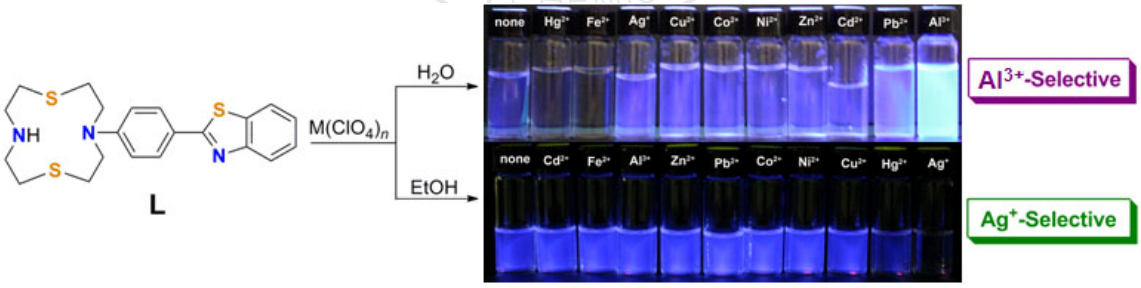
발표종류: 포스터, 발표일시: 목 15:00~17:00

Benzothiazol-Attached Thiaaza Macrocycle as A Dual-Photophysical Probe Receptor: Solvent Effects

박선홍, 이소영, 이심성

경상대 화학과

A benzothiazolyl-group-bearing thiaaza-macrocycle L was synthesized and its sensing properties for metal ions were investigated through two channels (color and fluorescence). For example, Al(III) resulted in the largest λ_{max} change in the absorption spectra of the ligand while no shift was observed on addition of a range of other metal ions in water. L also showed Al(III) selectivity in terms of its fluorescence enhance effect relative to other metal ions in water. However, in ethanol, L exhibited Ag(I)-induced fluorescence quenching behavior. The observed solvent effect on the metal ion sensing can be explained due to the strong solvation of Ag(I) in water and that of Al(III) in ethanol.



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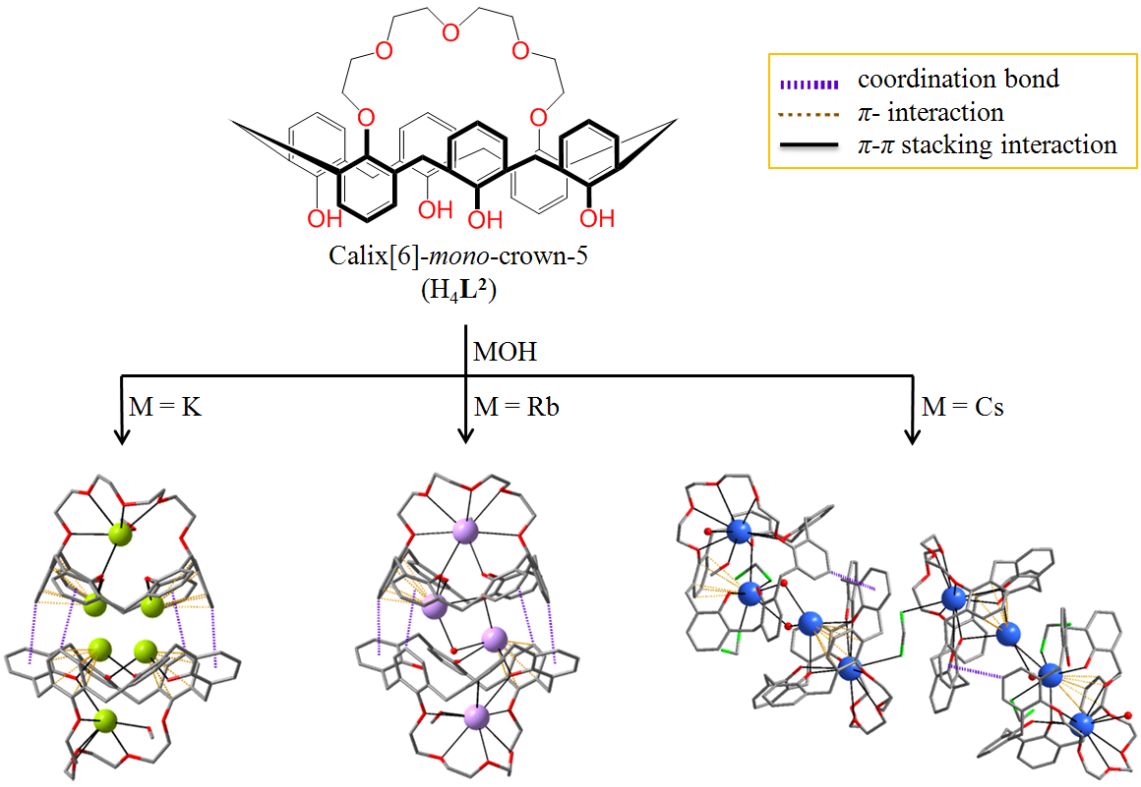
발표종류: 포스터, 발표일시: 목 15:00~17:00

Calixcrown Capsules: Homo & Heteromulti-Nuclear Alkali-Metal Complexes of Calix[6]-*mono*-crowns with Multiple Contacts

박인혁, 박기민, *Jacques Vicens, 이심성

*경상대 화학과 *IPHC-ULP-ECPM-CNRS URA 7178, 25 rue Becquerel, F-67087 Strasbourg Ce´dex, France*

Assembly of multinuclear alkali metal ion complexes of calix[6]-*mono*-crowns(n=4: H_4L^1 and n=5: H_4L^2) which can be denoted as '*n*M+@*capsule*' are reported. In each complex, the two facing calix[6]-*mono*-crown units interact pairwise via edge-to-face π-π stacking, adopting a '*capsule*' conformation. We also confirmed that the metal cations are stabilized by multiple contacts such as O(ether)-cation bond, O^-(phenolate)-cation bond, cation-π coordination, cation-solvent coordination and π-π stacking interaction. As we understand, the calixcrown capsules are new system that can recognize the multinuclear species via multiple contacts.



1, $6K^+$@capsule **2**, $4Rb^+$@capsule **3**, $[(4Cs^+@capsule)_2(\mu_2\text{-}CH_2Cl_2)]$

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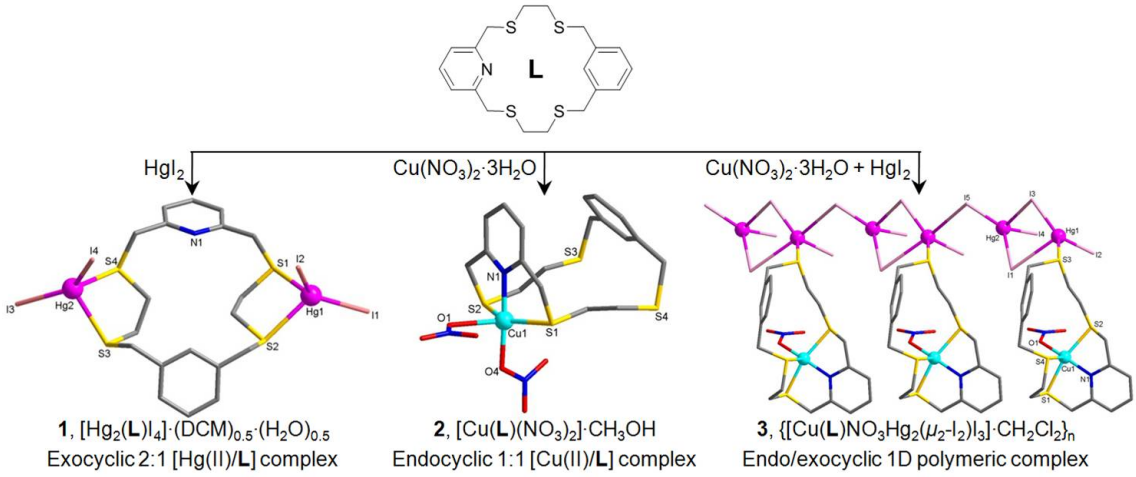
Synthesis of An NS_4-Macrocyclic Ligand and Its Supramolecular Copper(ll), Mercury(ll) and Silver(l) Complexes

이은지, 김현지, 이심성

경상대 화학과

We proposed a ditopic macrocycle L which employs an NS_2 donor set in one side to accommodate one metal cation in the cavity and the two sulfur donors as bridgeheads for the exocoordination. The NS_4-macrocycle (L) and its mono- and heterobinuclear supramolecular complexes have been synthesized and structurally characterized. Reaction of HgI_2 with L afforded an exo-coordinated dinuclear complex of 1 (see below). Reaction of $Cu(NO_3)_2$•$3H_2O$ with L afforded a dark green colored endocyclic 1:1 copper(II) complex of 2, in which the metal ion is accommodated inside the macrocyclic cavity (see below). Interestingly, reaction of L with the mixture of HgI_2 and $Cu(NO_3)_2$•$3H_2O$ (1 equiv plus and 1 equiv) afforded a 1D array of 3, in which endocyclic copper(II) complexes are linked with exocyclic mercury iodide cluster backbone via Hg-S bonds (see below). On the other hands, reaction of HgI_2 and CuI with L afforded heteronuclear complexes of formula $\{Hg_2I_6(L)_2[(\mu_2\text{-}Cu_2)]\bullet CH_3CN\}_n$, in which each ligands are bridged by μ_2-Cu_2.



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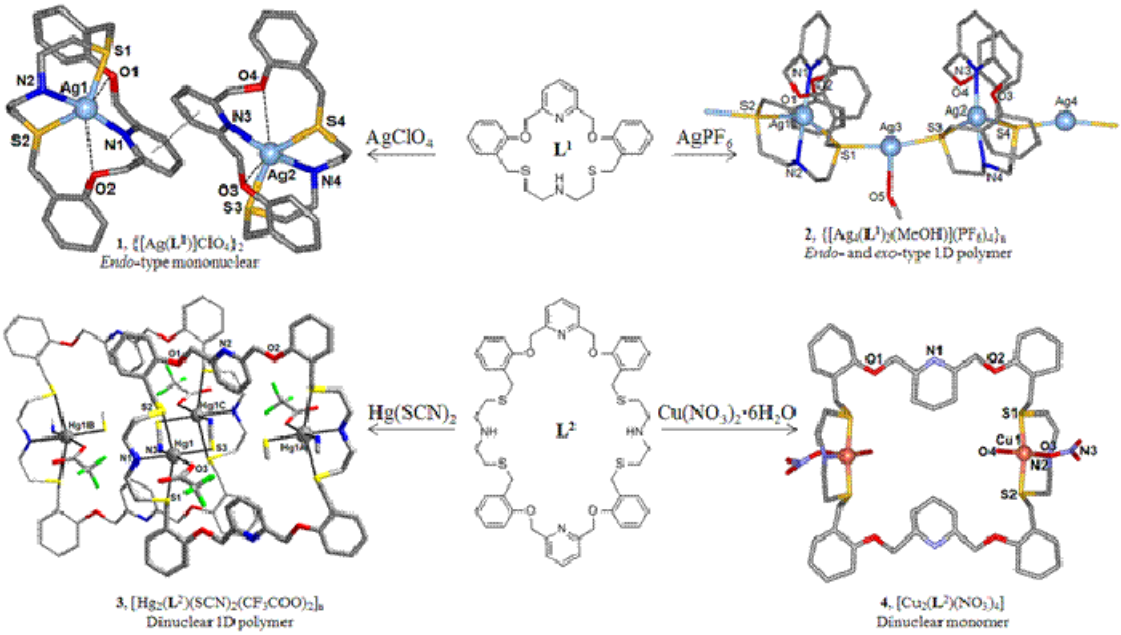
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Diazaoxathia Macrocycle Derivatives and Their Soft Metal Complexes: Dinuclear Complexes of the Extra-Large (XL) 40-Membered Macrocycle

정다람, *Rie Chamura, *Yoichi Habata, 이심성

*경상대 화학과 *Department of Chemistry, Faculty of Science, Toho University, 2-2-1 Miyama, Funabashi, Chiba, 274-8510, Japan.*

The coupling reaction of dichloride with N-Boc dithiol led to both 20-membered $N_2O_2S_2$ (L^1) and 40-membered $N_4O_4S_4$ (L^2) macrocycles via [1+1] and [2+2] cyclizations, respectively. Since the isolation of free L^2 were not successful, undertook the preparation of the L^2 complex directly from the mixed macrocycles. The reactions of L^1 with $AgClO_4$, $Hg(ClO_4)_2$ and $Cu(ClO_4)_2$•$6H_2O$ afforded endo-type mononuclear complexes. Meanwhile, reactions of L^1 with CuI and $AgPF_6$ gave 1D polymeric complexes. Interestingly, an extra-large (XL) 40-membered $N_4O_4S_4$ macrocycle (L^2) obtained through the [2+2] cyclization as a minor product has allowed to prepare and isolate its dimercury(II) (3) and dicopper(II) (4) complexes. In dimercury(II) complex 3, two mercury(II) ions occupy each NS_2 binding site in the extra-large cavity of L^2. These dinuclear complex units are further doubly linked by two bridging thiocyanate ions, adopting a 1D stair-way type polymeric array. In dicopper(II) complex 4, two copper(II) ions simply occupy each NS_2 binding site. As we understand, the synthesis and structural characterization of 1D type binuclear complex as large as 40-membered macrocycle has not been reported. Currently we are investigating not only the separation of the XL macrocycle but also the preparation of its new metallo-supramolecules such as cascade and catenated complexes with some guests.



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일시: 2010년 10월 14~15일(목~금) 2일간
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Synthesis of EDTA surface capped water-dispersible ZnS:Mn nanocrystals

이재욱, 황청수

단국대 화학과

The preparation of semiconductor nanocrystals ZnS:Mn-EDTA quantum dots were described. ZnS:Mn-EDTA nanocrystals were synthesized via two methods. One method was injecting zinc sulfate, manganese sulfate, sodium sulfide, solvent (H2O) and then directly mixing capping-ligand EDTA. The other method was the thermal decomposition reaction of their corresponding organometallic precursors (diethylzinc, bis(acetylacetonato)- manganese(II), and hexamethyldisilathiane) in a coordinating solvent (TOP/TOPO) mixture. And the organic surface capping agents were substituted with EDTA molecules to impart hydrophilic surface properties to the resulting nanocrystals. The optical properties of the water-dispersible nanocrystals were analyzed by UV-visible and room temperature soultion photoluminescence (PL) spectroscopy. The powders were charactererized by X-ray diffraction (XRD), high resolution transmission electron microscopy (HR-TEM), and elemental compositions confirmed by EDXS.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

pH-Controlled Synthesis of CdS Nanospheres by Hydrothermal Reaction

전영진, *이명한

*건국대 응용화학과 *건국대 첨단응용학과*

CdS 는 상온에서 2.4eV 의 띠간격을 갖는 Ⅱ-Ⅵ족 반도체이다. CdS 의 탁월한 발광 특성과 광화학적 특성은 태양전지, 광학 다이오드, 레이저, 광학, 의학, 전기, 촉매 등 여러 분야에서 연구되고 있다. 본 연구에서는 $Cd(NO_3)_2$ 와 sulfur 공급원으로 L-cysteine 을 섞어 수열반응법으로 합성하였다. 특히 pH 에 따라 CdS particle 의 형태가 달라짐을 확인할 수 있었다. pH 12 에서 합성된 CdS 는 약 400 nm 정도의 크기를 갖는 구형임을 확인하였다. 발표에서는 이를 SEM, XRD, IR, Raman, TGA 를 이용한 성질 규명과 반응메커니즘에 대해 논의하고자 한다.

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A Simple Route for Fabricating Silicon Nanowires from Block Copolymer Thin Films

최신호, *박수진

*울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부*

Research of method made sub-30nm silicon nano wire by nano-patterned block copolymer film and Reactive Ion Etching. In the research, regulated micelle size and interval by control of Molecule weight of block copolymers. For make the 2D array micelle, Spin coated polystyrene-b-poly(2-vinylpyridine) block copolymer in toluene dissolved in selective solution as toluene Xylene on the sample. The part is polystyrene that overlap each other in Corona region, this part etched by RIE(Reactive Ion Eching). Deposition metal catalyst as Silver and Gold about proper thickness after Silicon wafer etched by electroless metal deposition. Surface of wafer etching by the reaction of deposited metal as silver and mixed solution (HF(Hydrofluoric Acid)+H2O2(Hydrogen peroxide)). it make different form of etching depend on deposition metal. By the method of research, it make silicon nano-wires.

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Facile synthesis of Bismuth CPs 2D Sheets under Hydrothermal Condition

전영진, *한성준

*건국대 응용화학과 *건국대 첨단응용학과*

배위고분자는 가스저장, 촉매, 이온교환, 분리, 약물개발등 응용성이 높아 상당한 주목을 받고 있다. 배위고분자는 사용하는 금속, 리간드의 선택, 반응 조건을 조절하여 형태의 변화를 통제 할 수 있다. 본 연구에서는 $Bi(NO_3)_3$ 와 L-methionine 을 이용하여 수열반응 조건하에 pH, 온도, 반응시간 등을 조절하여 Bi(L-methionine) 배위고분자를 일정한 크기를 갖는 2D sheets 형태로 합성하였다. pH 조절과 반응시간, 온도등의 변화에 따른 형태, 구조의 변화를 SEM, XRD, IR 등을 이용한 실험의 결과를 발표하고자 한다.

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Molecular Magnetism and photoluminescence of transition metal complexes with organic ligand including pyridyl and ethanol moieties

신종원, 로투산카라라오, *조현정, *서유림, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

Six transition metal complexes, $[Fe_4(bpaeO)_2(CH_3O)_2(N_3)_8]$ (1), $[Co_3(bpaeO)_2(N_3)_4(NO_3)](NO_3)$ (2), $[Fe(bpaeOH)(NCS)_2]$ (3), $[Co(bpaeOH)(NCS)_2]$ (4), $[Mn(bpaeOH)(NCS)_2]$ (5), and $[Mn(bpaeO)(N_3)_2]$ (6), have prepared and characterized by various spectroscopies. Complex 1 shows both ferromagnetic and antiferomagnetic couplings between the iron(III) ions within the tetranuclear unit, while 2 is a mixed-valence trinuclear cobalt(II/III) complex and also shows high-spin cobalt(II) in X-band EPR spectrum. Furthermore, 3 and 4 with thiocyanate ions exhibit high-spin states in the temperature range 2 to 300 K. Manganese(II) complex 5 with one bpaeOH and two thiocyanate ions and manganese(III) complex 6 with a deprotonated bpaeO and two azaide ions have different oxidation states depending on the type of binding anions. In this poster, we will explain the detailed preparation, crystal structure, magnetic properties, EPR spectra, photoluminescent behaviors as well as interesting coordination chemistry.

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Metal Complexes with Cyclam and Functionalized TTF (tetrathiafulvalene) Ligands : Syntheses and characterization

이주은, 김유정, 이홍인

경북대 화학과

Charge-transfer salts, composed of TTF (tetrathiafulvalene) and metal ions, exhibit interesting electric and magnetic properties. We have synthesized two types of TTF derivatives; one is functionalized with cyano groups (tetracyanotetrathiafulvalene) and the other with carboxylate groups, BCDT-TTF [Bis(4(5)-carboxy-1,3-dithiolidene)]. We adapt macrocyclic building blocks, such as metal-cyclam, to synthesize multi-dimensional metal-cyclam-TTF complexes. Metal-cyclam-TTF complexes are characterized by various analytical methods including EA (Elemental Analyzer), EPR (Electron Paramagnetic Resonance), IR and UV.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and characterization of novel (*μ*-oxo)diiron(III) complexes

신종원, 로투산카라라오, *조현정, *서유림, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

Much effort has been directed towards the chemistry of binuclear iron(III) complexes with oxo-bridged cores due to their relevance to the magnetic interactions between the two iron(III) centers and biological systems such as the iron catalases. Owing to the viewpoint we have synthesized two dinuclear iron(III) complexes with an oxo-bridged, $[Fe^{III}(bpaeOH)(C_2O_4)O(C_2O_4)(bpaeOH)Fe^{III}]$ (1) and $[Fe^{III}(tpa)(N_3)_2O(N_3)_2(tpa)Fe^{III}]$ (2) from the reaction of *N*,*N*-bis(2-pyridylmethyl)-2-aminoethanol (bpaeOH) and tris(2-pyridylmethyl)amine (tpa), respectively. The crystal structures of 1 and 2 have been determined by single-crystal X-ray analysis. Herein, the detailed preparation, crystal structure, magnetic properties of 1 and 2 will be presented.

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Synthesis of Novel Germanium Precursors for GST Thin Film Deposition using ALD/CVD

김효숙, 박보근, 김창균, 정택모

한국화학연구원 화학소재연구단

Germanium complexes have been studied due to potential application in Ge2Sb2Te5 (GST) thin films for next generation nonvolatile phase-change random access memory (PRAM). The germanium precursors for application in thin films are thermally stable and highly volatile and lessen incorporation of impurities. We synthesized novel germanium precursors for GST thin films using ALD/CVD process and characterized by NMR, FT-IR, elemental analysis, and TGA.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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A New Thin Film Material: Metal-Organic Porous Material Thin Films and Their Dynamic Breathing Property

윤민영, *이다미, 김영국, 김기문

*포항공과대 지능초분자 연구단, WCU 첨단재료과학부, 화학과 *포항공과대 지능초분자 연구단, WCU 첨단재료과학부*

Metal-organic porous materials (MOPMs) are one of the hottest materials because of their wide range of applications, such as in catalysis, separation, and storage. Although thin films of MOPMs would have many interesting properties and applications, the synthesis of well ordered MOPM thin films in a large area has yet to be achieved. Here we present a new family of the thin film materials through epitaxial growth of MOPMs on a self-assembled monolayer. The resulting thin films were characterized by various techniques including in plane and out of plane X-ray scattering, IR, and SEM. In addition, the dynamic breathing property of the MOPM thin film induced by solvent exchange will be presented.

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Novel Pd catalysts for the Emulsion Copolymerization of functionalized norbornene with bulky olefins

이응준, 안명용, 이익모

인하대 화학과

Polynorbornene has been a good candidate for the optical devices working in the short wavelength but brittleness prevented this material from further applications. Copolymerization of functional norbornenes with norbornene or dicyclopentadiene(DCPD) would be a possible method for the improvement of properties of norbornenes. Many Pd or Ni complexes are known to polymerize norbornene but they are sensitive to the polar groups of functional norbornenes. In our search for the active catalytic systems for the polymerization of functional norbornenes, we found that Pd complexes with β-diketiminates were quite soluble in common organic solvents but highly stable in water. Emulsion copolymerization of functional norbornenes with bulky olefins has been achieved in the presence of Pd complexes with β-diketiminates and the effects of various reaction parameters have been investigated.In this presentation, preparation and copolymerization behaviors of an efficient catalytic system will be discussed.

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DCPD vinyl addition polymerization by using reaction injection molding (RIM)

안명용, 이응준, *황운성, **성익경, 이익모

*인하대 화학과 *(주)코오롱 기술연구소 **코오롱유화(주) 기술연구소 연구1팀*

DCPD is an economically interesting monomer since it is a byproduct in the petrochemical industry (C5 fraction) and is cheap and readily available, at least as a technical grade. It has been used, for example, to produce objects by reaction injection molding (RIM). Poly DCPD has mechanical properties similar to engineering thermoplastics and commonly obtained by ring-opening polymerization. We found that polyDCPD can be obtained by vinyl addition polymerization by Pd complexes and this would show different properties from those obtained from ROMP. The properties of polyDCPD and effects of reaction parameters on the properties of polyDCPD will be discussed.

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Synthesis of new tridentate ligands containing β-diketimines

윤샛별, 이병기, 이익모

인하대 화학과

Recently, multidentate ligand has been drawn a lot of attention due to possible multinuclear complex structure with high stability. Since the start of olefin polymerization by Ziegler-Natta catalysts, extensive researches have been performed to find new organometallic compounds catalytically active in polymerization. Constrained geometry catalysts (CGCs) have been reported to be very active in the polymerization of olefins. It also reported that β-diketiminate ligands with bulky substituents such as isopropyl or t-Bu could coordinate to the metal in an η5 modes. In order to find out if new CGC catalysts with β-diketiminates for Cp or Cp*, we synthesized various β-diketiminate ligands with tailing amines by nucleophilic substitution of SiMe2Cl2. The effect of various reaction parameters on the preparation of tridentate ligands will be discussed.

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Preparation of nanocrystalline TiO_2 by microwave-assisted hydrothermal reaction and the effect of TiO_2shape on the photovoltaic effeciency

최민식, 이익모

인하대 화학과

A new synthetic process assisted by microwave has been reported for the easy control of structural shapes and sizes of nanocrystalline TiO_2. Efficiency of dye-sensitized solar cell (DSSC) based on TiO_2 has been an obstacle for the further application. It has been known that spherical TiO_2 particles should be in the range of 15 to 20 nm for the maximum efficiency and P25 has been used as a standard in this kind of experiments. For the higher efficiency of DSSC, scattering layer method has been introduced recently. The principal of scattering layer method is reuse of light by the reflection of the light transferred through TiO_2 electrode to the electrode again. A larger particles than ones in the conventional cell is expected to show higher efficiency. It is found that TiO_2 with Hollow sphere (HS) and hollow tube (HT) shapes obtained by microwave-assisted hydrothermal reactions in our previous research showed higher efficiency as expected by application of scattering layer method. This can be rationalized by the larger surface areas and more dyes adsorbed in the HS and HT particles containing voids in their bodies. This overall procedure with easy scale-up is simple, reproducible, and relatively inexpensive.

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Syntheses and Optical properties of the Water-dispersible ZnS:Mn nanocrystals Surface capped by Polyethylene glycol

김송이, 황청수

단국대 화학과

Water-dispersible ZnS:Mn nanocrystals were synthesized by capping the nanocrystals' surfaces with PEG (polyethylene glycol) molecules of three different molecular weights (g/mol): 1,500: 4,000: 10,000. The resulting nanocrystal powders were characterized by XRD, HR-TEM, and EDXS. The optical properties of colloidal ZnS:Mn-PEG nanocrystals were measured by UV/Vis and solution photoluminescence (PL) spectroscopies. The solution PL spectra showed broad emission peaks around at 600nm with PL efficiencies in the range of 1.8 to 5.3%. Among the capping ligands, PEG-10,000 yielded the best luminescence property for the ZnS:Mn nanocrystals. The x-ray diffraction (XRD) measurements showed that the nanocrystals have the structure of wurtzite. Finally, particle sizes for the PEG capped nanocrystals were measured from the HR-TEM images to be in the range of 2.9 to 3.4nm.

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

Three-dimensional bimetallic complex built with iron(II) metalloligand exhibiting magnetic property and porosity

유대원, 홍창섭

고려대 화학과

A three dimensional porous complex, $[Fe(Tt)_2Cu_6(isophthalate)_6]$ [Tt=tris(1,2,4-triazolyl)borate], was prepared by a solvothermal reaction with Cu(II) ion, isophthalic acid, and $Fe(Tt)_2$ in mixed solvent of DMA, H_2O, and MeOH. This complex contains the metalloligand $[Fe(Tt)_2]$ with six exodentate sites and Cu(II) ions are formed a paddle-wheel type cluster. Axial positions of the paddle-wheel cluster are occupied by nitrogen atoms from metalloligands. We will present the detailed structure, sorption and magnetic properties in the presentation.

한국화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-104**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, crystal structures, and magnetic properties of cyano-bridged $Mn^{III}M^{V}$ (M = Mo, W) heterometallic chains with slow magnetic relaxations

윤정희, 유대원, 최상엽, 홍창섭

고려대 화학과

Two new one-dimensional complexes, $\{[Mn(5\text{-}Brsalcy)][M(CN)_8]\}[Fe(CH\text{-}3,5Me_2pz_3)_2]\cdot xMeOH\cdot yH_2O$ [M = Mo (1) and W (2)], have been successfully obtained and both complexes are almost structurally identical. The crystal structures contain one-dimensional bimetallic chains constructed from $Mn^{III}Mo^{V}$(or $Mn^{III}W^{V}$) properties show the obvious existence of antiferromagnetic interactions between M^{V} and Mn^{III} ions, particulary leading to a sudden rise of $\chi_m T$ at low T for 1. Interestingly, slow magnetic relaxations are clearly visible in 1 and 2, to single-chain magnet behavior attributable. Detailed structural and magnetic studies will be given in the presentation.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-105**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Syntheses, crystal structures, and magnetic characterizations of Fe^{III}-Mn^{III} bimetallic complexes formed by a newly designed *fac*-Fe tricyanide

조경진, 유대원, 홍창섭

고려대 화학과

Reaction of $[(Tp^{memt3})Fe^{III}(CN)_3]^-$ with respective Mn(III) Schiff bases led to the formation of two tetrameric complexes, $\{[Mn^{III}(5\text{-MeOsalen})]_2[Fe^{III}(Tp^{memt3})(CN)_3]_2\}$ (1) and $\{[Mn^{III}(5\text{-Clsalen})]_2[Fe^{III}(Tp^{memt3})(CN)_3]_2\}$ (2). The crystal structures show that the axial sites of the central Mn dimeric unit linked by phenoxide oxygens from the Schiff bases is completed by two terminal Fe tricyanides. Magnetic measurements reveal that overall antiferromagnetic couplings are operative between spin centers for 1 whereas overall ferromagnetic interactions occur in 2. Structural and magnetic characteristics of the present compounds will be discussed in a more detail.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-106**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A 3D chiral metal-organic framework constructed from achiral ligands

방원주, 홍창섭

고려대 화학과

In recent years, the design and controlled assembly of coordination frameworks based on metal centers and multifunctional bridging ligands are of great interest due to their versatile architectures, topologies as well as potential applications in various areas, such as heterogeneous catalysis, gas adsorption, molecular storage, separation, and fluorescent sensing. We have synthesized a 3D metal-organic framework by reacting cadmium nitrate, 1,3,5-Tri(4-carboxyphenoxy)benzene (H_3TCPB), and 4,4'-bpy. In this framework, 2D layers formed by cadmium divalent cations and TCPB are pillared via 4,4'-bpy, leading to a 3D porous network. Interestingly, it is noted that a chiral space group, $P2_1$ is encountered in spite of the introduction of an achiral ligand. SBUs consist of three Cd^{II} atoms, of which one is octahedrally coordinated with six different carboxylate oxygens and two have pentagonal bipyramidal geometries with three different carboxylate oxygens, 4,4'-bpy and one H_2O molecule or one DMF molecule. The framework is highly stable up to about 400℃. We will discuss detailed structure and gas sorption studies in the presentation.

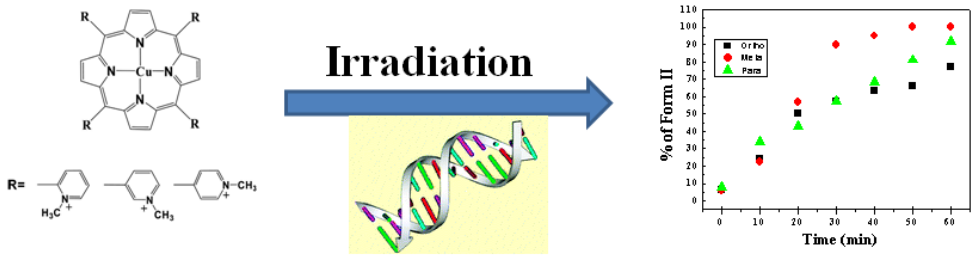
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-107**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Photo induced cleavage activity of Cu(II)-meso-tetrakis(n-N-methylpyridiniumyl)porphyrin

프리아, *장윤정, *김석규, **이효선

*경북대 화학과 *영남대 화학과 **경북대 자연과학대학 화학과*

Photoinduced cleavage of P-Gem 50 DNA with well known Cu′ TMPyP complexes has also been examined by agarose gel electrophoresis. The complexes are successfully promotes the cleavage of p-Gem 50, producing single DNA strand breaks. The amount of conversion of supercoiled form (SC) of plasmid DNA to the nicked circular form (NC) depends on the duration of irradiation of the complex with DNA. The maximum rate of conversion of the supercoiled form to the nicked circular form occurred in Meta derivative. The photocleavage activity of the porphyrins diverged on the structural characteristics of the porphyrins such as the position of the side chain on the porphyrin ring. Meanwhile, the binding properties of P-gemDNA with these porphyrins have been comparatively investigated and compared also with that of the CT-DNA binding ability.



THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-108**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Comparison of binding stoichiometry of [Ru(1,10-phenanthroline)2dipyrido[3,2-a:2',3'-c]phenazine]$^{2+}$and its bis-derivative to DNA

WANGWEI, 이현미, *이동진, 장윤정, 김석규

*영남대 화학과 *경일대 공업화학과*

A new bis-Ru(II) complex, in which two [Ru(1,10-phenanthroline)$_2$dipyrido[3,2-a:2',3'-c]phenazine]$^{2+}$ were tethered by a 1,3-bis(4-pyridyl)propane linker, were synthesized and its binding mode and stoichiometry to DNA was investigated by optical spectroscopy including linear dichroism (LD) and fluorescence intensity measurement. The magnitude of the negative reduced LD signal of the *bis*-Ru(II) complex in the dipyrido[3,2-a:2',3'-c]phenazine (DPPZ) ligand absorption region appeared to be similar compared to that in the DNA absorption region, which is considered to be a dignostic for DPPZ ligand intercalation. The binding stoichiometry measured from its LD magnitude and inhanced fluorescence intensity corresponds to one ligand per three DNA bases, effectively violating the nearest neighbouring site exclusion model for classical DNA intercalation. This observation is in contrast with monomer analogue [Ru(1,10-phenanthroline)$_2$dipyrido[3,2-a:2',3'-c]phenazine]$^{2+}$, which is saturated at the DPPZ ligand to DNA base ratio of 0.25, or one DPPZ ligand per four nucleobases.

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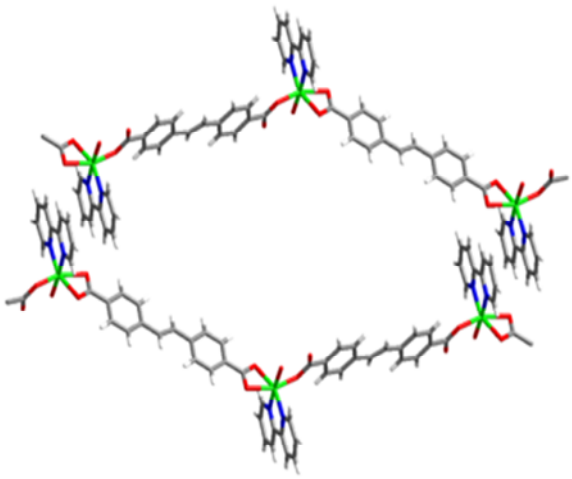
장소: 대구엑스코
발표코드: **INOR.P-109**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of Metal-Organic Coordination Plymers with Large Internal Void Space from 1D Coordination Polymers

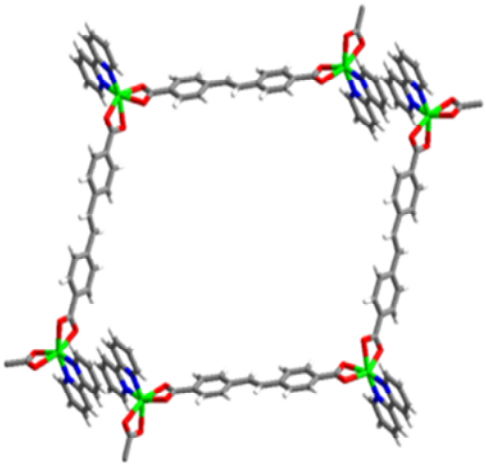
박경세, *김현욱, **이강호, ***이하진, 유수창, *김기문

*군산대 화학과 *포항공과대 화학과 **경북대 화학과 ***한국기초과학지원연구원 전주센터*

The two 1D chains dictated by solvent system were prepared by solvothermal reaction. A single-crystal X-ray analysis reveals that 1 is a 1-D zigzag polymeric coordination chain with molecular formula of [Co(SDA)(Bipy)(H_2O)]•0.84DMF•2H_2O and that 2 is also the 1-D zigzag polymeric coordination chain with molecular formula of [Co(SDA)(Bipy)]•HH_2O. Interestingly, intermolecular bipy units in 1 and 2 adopt π- π stacking interactions between neighboring undulating 1D chains resulting formation of 2D networks which further extend into 3D supramolecular frameworks individually through hydrogen bonding for 1 and π- π stacking interactions for 2. Thermogravimetric analysis (TGA) were performed to evaluate the thermal stability of these compounds. Magnetic properties of 1 and 2 were also investigated by using a Squid magnetometer (Quantun Design, MPMS 7).



1



2

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-110**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

EDTA surface capped water-dispersible ZnSe nanoparticle

이상민, *황청수

*단국대 무기화학실험실 *단국대 화학과*

We synthesized ZnSe-EDTA nanoparticles having luminescence which ranges in wavelength from 340 to 430nm. ZnSe-EDTA nanoparticles were synthesize via two methods. One method, precursors(ZnSO4, Na2SeO4, Na2EDTA, NaOH) in a water solvent mixture, that was reacted via autoclave system. Another method, precursors((Et)2Zn, SeTOP) in a hot coordinating solvent (TOP/TOPO) mixture. The organic surface capping agents were substituted with EDTA molecules to impart hydrophilic surface. Water-disperse nanoparticles were analyzed by high resolution transmission electron microscopy (HR-TEM), and confocal laser scanning microscopy (CLSM).

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of a Ru(Ⅲ) Complex Containing Tris[2-(1-pyrazoyl)ethyl]amine (Tpea) Ligand : Reactivity toward Carminic Acid

조장훈, 김은지, 이홍인

경북대 화학과

We have synthesized a Ruthenium(III) complex containing a tripodal tris[2-(1-pyrazoyl)ethyl]amine (=Tpea) ligand,[Ru(III)(L)Cl_2]ClO_4(L=Tpea). In this research, the reactivity of the Ru complex toward carminic acid has been investigated using hydrogen peroxide and tert-butyl hydroperoxide as oxidants. We describe here the reaction monitored by UV-VIS, EPR, and CV at various pH conditions.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
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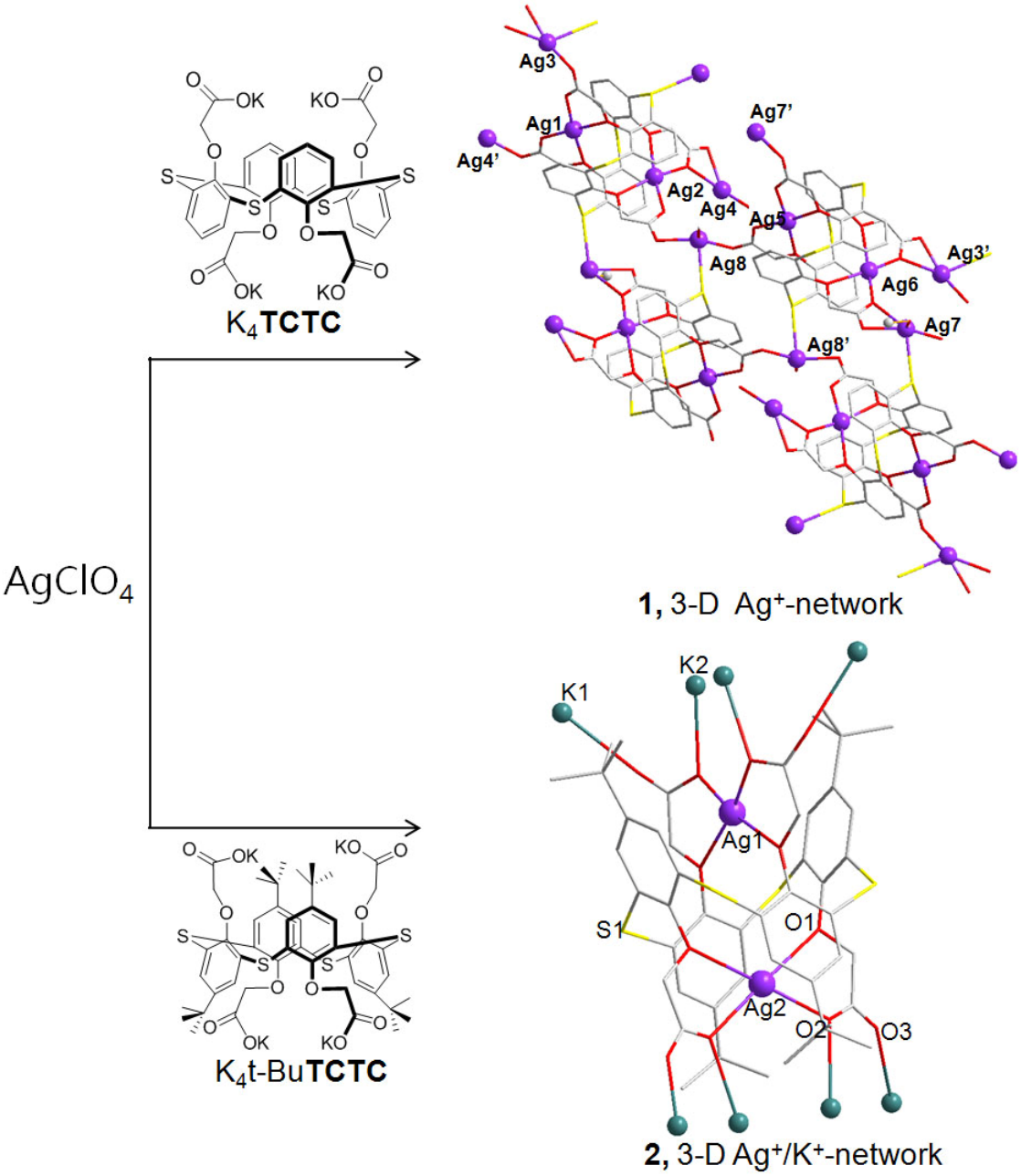
발표코드: **INOR.P-112**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Network Complexes of Thiacalix[4]arene Tetracaboxylate

김기환, 박선홍, 박기민, 이심성

경상대 화학과

Thiacalix[4]arene tetracarboxylate potassium salts (K_4TCTC and K_4*t*-BuTCTC) were prepared as a vesatile building block for the construction of coordinative networking species. Reaction of K_4TCTC with $AgClO_4$ afforded a potassium(I)-free 3-D network complex 1, $[Ag_8(TCTC)_2]_n$, in which one 1,3-alteranate thiacalix[4] scaffold with tetracarboxylate unit stabilizes eight silver by multiple interactions. The potassium(I) ion were found to replace the silver(I) ion in 1 and bind to sulfurs and oxygens giving the infinite 3-D structure. On the other hands, the parallel reaction with K_4*t*-BuTCTC afforded the expected heteronuclear network complex 2.


K4TCTC
AgClO4
Ag3
Ag1
Ag4'
Ag7'
Ag2
Ag4
Ag5
Ag8
Ag3'
Ag6
Ag7
Ag8'
1, 3-D Ag+-network
K4t-BuTCTC
K1
K2
Ag1
S1
O1
Ag2
O2
O3
2, 3-D Ag+/K+-network

일시: 2010년 10월 14~15일(목~금) 2일간
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발표코드: **INOR.P-113**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of CdTe quantum dotsthrough a simple sonochemical method

황차환, 심일운

중앙대 화학과

Cadmium Telluride quantum dots have been synthesized under high temperature condition using organic solvent or aqueous solution for long reaction time. But under the MBSL(multibubble sonoluminescence) condition, CdTe quantum dots were synthesized rapidly in mild condition. For the synthesis, we used cadmium chloride, tellurium powder and TOP/TOPO. The particle size was controlled by changing reaction time. The prepared CdTe quantum dots were examined by XRD, Uv-vis, FS and TEM.

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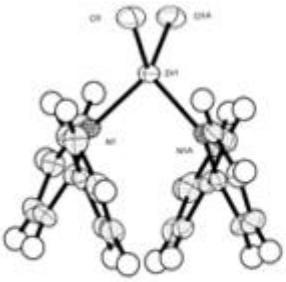
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of metal complexes to model carbonic anhydrase system

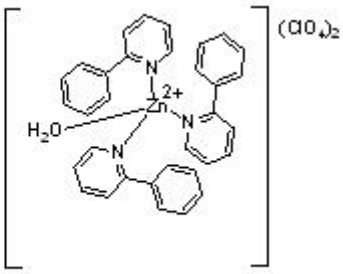
D.Sivanesan, *윤성호

*국민대 화학과 *국민대 생명나노화학과*

Carbonic anhydrase is a zinc enzyme with the essential role of catalyzing the reversible hydration of carbon dioxide. The active site of the enzyme is a pseudo tetrahedral zinc center coordinated to three histidine group and a water molecule [(His)3Zn-OH2]2+. Currently, we aim to synthesis new zinc complexes to mimic the carbonic anhydrase system. There are very few compounds, which can convert carbon dioxide to bicarbonate efficiently. The compound shown in figure I, was prepared and its derivatives will be synthesized. Herein, we report the synthesis, pKa values and conversion rate of CO2 to bicarbonate using metal complexes.



$C_{22}H_{18}Cl_2N_2Zn$



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-115**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Facile Preparation of Ag Nanowires in One-Pot Route

이경훈, *주본식, *윤성호

*국민대 나노과학기술협동과정 *국민대 생명나노화학과*

One-dimensional nanomaterials in range of 1-100 nm have been one of the hottest issues because they have unique properties and a promising potential in various fields, such as an element of solar cell, porous electrode, and transparent conducting film. Among metals, silver has been extremely studied because of its excellent electrical and thermal conductivities. Many groups have shown well synthesized one-dimensional Ag nanowires using physical template such as alumina or polymer membranes, meso porous materials, and carbon nanotube. However, employment of physical templates could cause a complicated process and limit of scale. To overcome these difficulties, a solution phase method should be needed without physical template. Younan Xia and his coworker demonstrated the technique to synthesize Ag nanowires in solution phase [1]. But this method also has a limitation in mass-production of Ag nanowires. To make up for this limit, we designed specific equipment to produce Ag nanowires easily and continuously by a syringe pump, micro mixer and modified stainless tube. With controlling reaction time, we found the condition, which can prepare Ag nanowires. We believe that Ag nanowires can be synthesized largely with the confirmed condition and constant injection of starting materials into the syringe pump.Acknowlegment : This study was supported by a grant from the Fundamental R&D program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea[1] Yugang Sun and Younan Xia, Adv. Mater. 2002, *14*, 833

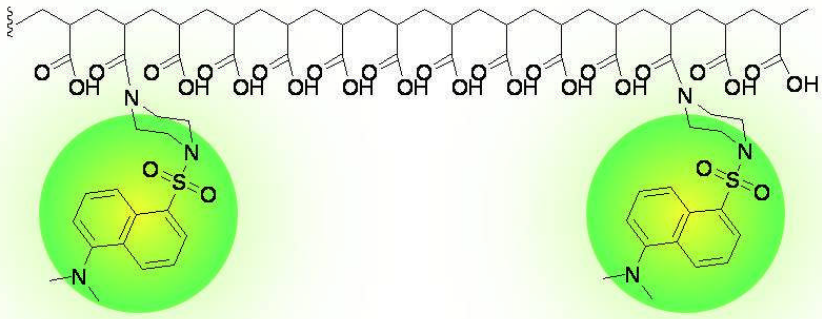
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-116**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Preparation of the Polymer-Bound Fluorophore to Prevent Self-Quenching Property in the Solid State

김지연, 윤성호

국민대 생명나노화학과

In Light Emiting Diode(LED), phosphors should be in the solid state with high Quantum Yeild (QY) most of organic phosphors are very fluorescent only in the solution state, because in the solid state they has very close intermolecular distance, resulting in decrease of optical efficiency through PL self-quenching phenomenon. To overcome such limit, we synthesized the polymer with fluorophore at regular intervals to increase the intermolecular distance. According to the Polymethyl metha acrylate (PMMA) bound Danzylpiperazine(Ds-pip), we observed differences of QY through the Photo Luminescence (PL) analysis.Acknowlegment : This study was supported by a grant from the Fundamental R&D program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-117**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

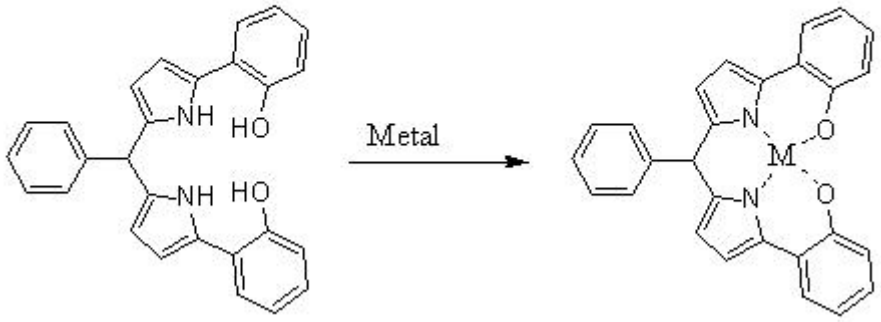
Synthesis of Hangman Ligands Containing Pyrrolylphenol Moiety

송혜선, 윤성호

국민대 생명나노화학과

In the recent studies of photosynthesis, the one of critical processes is the oxidation of water to a high valent metal oxo intermediate(M=O) for converting light energy into chemical energy 1 Especially, In the photosynthetic oxygen evolving complex(OEC) of photosystem II, the active site structure of the tetranuclear manganese cluster is of great important. We aim to synthesis new manganese complexes to mimic the manganes cluster in OEC. There are very few model complexes, which can acts as molecular catalyst for water oxydation. So, We designed novel hangman derivatived ligand, which can keep suitable distance for Mn-Mn interaction.Herein, we present detailed synthetic methods and structural studies of metal complexes [Mn2(1,8-bis[5,5'-bis(2-phenoxyl)pyrromethl]-hangman)]2 Acknowlegement: This work was supported by Korea Science and Engineering Foundation(KOSEF) grant funded by the Korean government(MEST). (2008-0060252)"

Scheme 1.



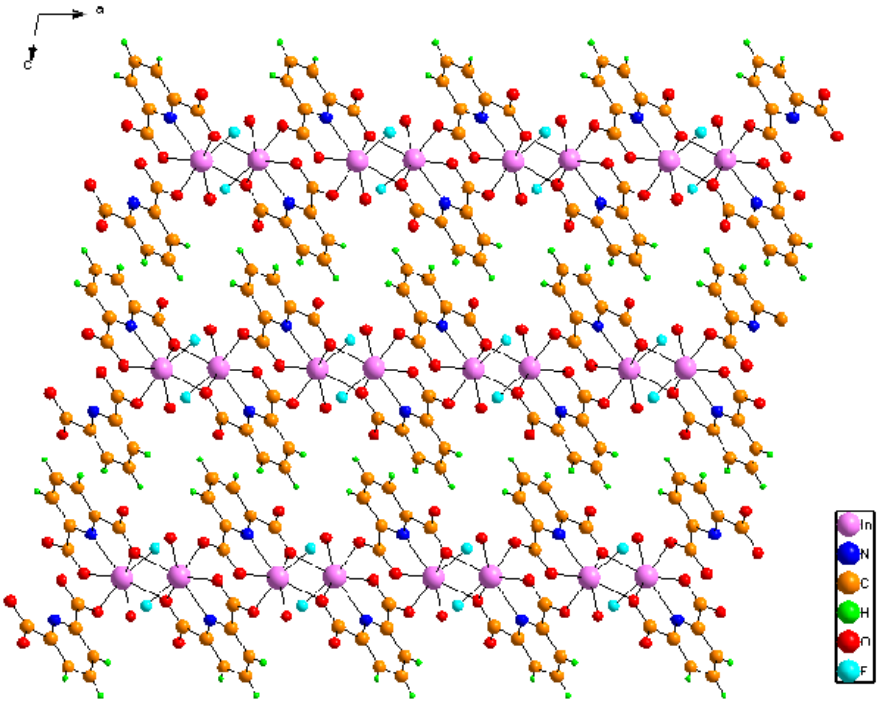
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **INOR.P-118**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, Crystal Structure, Exchange reactions, and Characterization of a New Layered Indium-Organic Framework Material, $In[NC_5H_3(CO_2)_2](OH_2)F$

김민경, 이동우, 옥강민

중앙대 화학과

A new layered Indium-organic framework material, $In[NC_5H_3(CO_2)_2](OH_2)F$ has been synthesized through a hydrothermal reaction. The In^{3+} cation with a variable coordination environment and the 2,6-pyridine dicarboxylate (pdc) organic linker were combined to create a new type of framework geometry. Single crystal X-ray diffraction was used to determine the crystal structure of the reported material. $In[NC_5H_3(CO_2)_2](OH_2)F$ has a novel layered structure consisting of InO_5NF polyhedra and the pdc organic linker. Within the layer, the material exhibits rectangular rings with strong hydrogen bonds. Exchange reactions of the coordinated water for other ligands in $In[NC_5H_3(CO_2)_2](OH_2)F$ turned out to be irreversible. Full characterization including infrared spectra, thermogravimetric analyses, elemental analyses, and gas adsorptions are also reported. Crystal data for $In[NC_5H_3(CO_2)_2](OH_2)F$: monoclinic, *I*2/*a* (no. 15), a = 12.929(3) Å, b = 7.8554(16) Å, c = 17.740(4) Å, β = 100.66(3), and Z = 8.



THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and characterization of Ir(III) complex based on o-carborane substituted phenylpyridine ligand

김태원, 이민형

울산대 화학과

Phosphorescent organic light-emitting diodes (PhOLEDs) based on heavy metal complexes have attracted great attention due to their high internal quantum efficiency up to 100% of a theoretical value by fully utilizing both singlet and triplet excitons. To increase the phosphorescent efficiency of Ir(III) complex, it is required to harvest and stabilize the triplet state of complex more effectively. To this end, we introduced an o-carborane moiety into phenylpyridine (ppy) ligand and synthesized novel Ir(III) complex supported by ppy ligand bearing an o-carborane subsitutient. Details of synthesis, characterization, photophysical and OLED properties of complex will be presented.

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Preparation and Characterization of Al2O3-CuO-ZnO/Co composite membrane on hydrogen permeation

임샛별, *홍태환, *김경일, 문보람, 유희정, 이영, 정미원

*성신여대 화학과 *충주대 신소재공학과*

The aim of this work was the hydrogen permeation measurements of Cermet (ceramic-metal composite) membranes using Al2O3-CuO-ZnO(ACZ). The ACZ, target materials, were synthesized from sol-gel process with aluminum isopropoxide, copper (Ⅱ) nitrate hemi (pentahydrate) Zn (Ⅱ) nitrate hexahydrate, and primary distilled water. Moreover, the Span 80 and CTAB (Cetyl trimethyl ammonium bromide) as the template block copolymers were added to ACZ composition mixture to increase surface area and catalytic activity. Cobalt helps to control hydrogen dissociation reaction and improved mechanical properties on membrane. Therefore, ACZ-Co composites membrane were prepared by hot press sintering (HPS). The ACZ synthesized powders were charaterized by Thermogravimetry-Differential thermal analysis (TG/DTA), X-ray Diffractometer (XRD), Field-Emmision Scanning Electron Microscope (FE-SEM), and Bruner-Emmett-Teller surface analysis (BET). Hydrogen permeability was characterized by Sievert's type hydrogen permeation membrane equipment.

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Fabrication and Evaluation of Thermo-electrical properties and hydrogen permeation on La doped CuO-ZnO-Al_2O_3 for Hydrogen Permeation membrane

문보람, 임샛별, 이영, 유희정, *홍태환, 정미원

*성신여대 화학과 *충주대 신소재공학과*

La doped CuO-ZnO-Al_2O_3 powders are prepared by sol-gel method with aluminum isopropoxide and primary distilled water as precursor and solvent. In this synthesized process, the obtained metal oxides caused to precursor such as copper(Ⅱ) nitrate hydrate and zinc nitrate hexahydrate were added. To improve thermal stability and to control surface areas of CuO-ZnO-Al_2O_3, lanthanum(Ⅲ) nitrate hexahydrate and sorbitan (z)-mono-9-octadecenoate(Span80) was used. The synthesized powders were calcined at various temperature. The characterization of the synthesized powders was measured XRD, FE-SEM, BET, TG-DTA, thermal diffusivity and electrical conductivity. Hydrogen permeation evaluations were examined at various temperatures under increasing pressure.

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Synthesis and Evaluation of Thermo-electrical properties on Al2O3 - CuO - CeO2 Composites for Hydrogen Permeation

유희정, 문보람, 이영, 임샛별, *홍태환, 정미원

*성신여대 화학과 *충주대 신소재공학과*

Ceria(CeO2) shows an excellent effect on the activity of the catalysts due to its outstanding oxygen storage capacity and the ease of the Ce(Ⅲ)-Ce(Ⅳ) redox cycle. It is well known that CeO2 is a modifier affecting the extent of dispersion of CuO and also improving resistance to the thermal loss of the alumina support. In the case of CuO-CeO2 system supported on Al2O3, the studies have shown that the addition of CeO2 increases considerably the activity of Cu supported on alumina. The object of this work was to study the effect of alumina supports in the activity of the CuO-CeO2 system. In this work, ACC composites are synthesized by sol-gel process. To improve surface area, organic additives are added to these composite. The ACC composites are characterized by Field-Emmision Scanning Electron Microscope (FE-SEM), X-ray Diffractometer (XRD), Thermogravimetry-Differential thermal analysis (TG/DTA), Bruner-Emmett-Teller surface analysis (BET) and hydrogen permeation test.

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Synthesis and Characterization of $CuO-CeO_2/SiO_2$ composites prepared via sol-gel method

이영, 임샛별, 문보람, 유희정, *홍태환, 정미원

*성신여대 화학과 *충주대 신소재공학과*

CuO/SiO_2 are active catalysts in several important reactions such as methanol steam reforming, dehydrogenation and ester hydrogenolysis. Moreover, ceria (CeO_2) is usually employed as a promoter for the other active metal component or as a support in the catalysts for the reactions involving the redox cycle. A study was focused on the effect of Cu/Ce/Si ratio on specific surface area and catalytic activities of the synthesized powder. $CuO-CeO_2/SiO_2$ composites were synthesized by sol-gel method with $Si(OC_2H_5)_4$ (TEOS), $Ce(NO_3)_3 \cdot 6H_2O$ and $Cu(NO_3)_2 \cdot 2.5H_2O$. The synthesized powder was characterized by X-ray Diffractometer (XRD), Field-Emmision Scanning Electron Microscope (FE-SEM) and Bruner-Emmett-Teller surface analysis (BET).

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Synthesis of Thickness-Controlled AlPO4-5 Films by Changing the Locations of Substrate in Synthetic Gel

최성은, 이진석

숙명여대 화학과

Aluminophosphate AlPO4-5, with AFI framework-type, consists of 12-membered ring channel with a diameter of 0.73 nm which are one-dimensional, electrically neutral and parallel to the c-axis of the crystal. These physical and geometrical properties allowed AlPO4-5 to be used in numerous applications. Moreover, the AlPO4-5 films with controlled microstructure are attractive for a number of applications, particularly for gas separation and catalysts in industry. Generally, crystal orientation, thickness and uniformity of the zeolite membranes determine their performance.Here, the aluminophosphate molecular sieve AlPO4-5 film was synthesized on glass substrate by simple one-step process. As controlling synthetic gel composition and reaction conditions, we were able to produce c-oriented AlPO4-5 film without seeds. Also, we presented a novel technique that was able to control thickness of AlPO4-5 film by changing the location of glass substrate through the comparison with one resulted from vertically placed substrate. The c-oriented molecular sieve films that have controlled thicknesses by this technique can be potentially useful for various applications.

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Synthesis of CdS/CdSe Nanowires via Solution-Liquid-Solid Mechanism

장희수, 이진석

숙명여대 화학과

Semiconductor CdS/CdSe nanowires(NWs) can serve as model systems for investigating the physical properties of one-dimensional(1D) nanostructures and have great potential for applications in electronics and photonic nanodevices. With numerous attractions arisen from their physical properties, CdS/CdSe NWs have been synthesized by vapor-liquid-solid(VLS) methods, but they have some limitations of high reaction temperature and low production.Here, we synthesized CdS/CdSe NWs via the solution-liquid-solid (SLS) mechanisms using bismuth (Bi) metal with low-melting point as a catalyst. In our synthetic processes, we use a Bi thin layer deposited on a substrate instead of Bi colloidal nanoparticles, because the catalyst-bound substrates is more easier to hold the produced NWs on the substrates than colloidal state ones. Particularly, we do not need to purify and reconcentrate reaction products for heterostructured NWs during the transfer of NWs from one reaction to another, and could clearly control the reaction time by picking up the substrates from solution.

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Nanocrystalline antimony oxide films for dye-sensitized solar cell applications

김지혜, 김승주, 장지연, *한치환

*아주대 에너지시스템학부 *한국에너지기술연구원 광전기소재연구센터*

Dye-sensitized solar cells (DSSC) are based on the dye sensitization of wide band gap semiconductors used in the form of mesoporous nanocrystalline films. Many attempts have been made to prepare and characterize the oxide semiconductors such as TiO_2, ZnO, SnO_2 and Nb_2O_5 for application to the DSSC . Antimony oxide also has a wide band gap. A new photoelectrode composed of Sb_6O_{13} nanoparticles with the size of 20-30 nm has been prepared via thermolysis of a colloidal antimony pentoxide tetrahydrate (Sb_2O_5•$4H_2O$) suspension. The change in composition and crystal structure of antimony oxides were monitored by means of powder X-ray diffraction and thermogravimetric method. On heating the antimony pentoxide tetrahydrate, the dehydration and reduction process successively proceed as follows. The former three compounds have pyrochlore structure, whereas the latter Sb_2O_4 has rutile structure. The energy band gap estimated from UV-Vis diffuse reflectance data decreases as the heating temperature increase to 450℃, then the energy band gap increases when the heating temperature is over 450℃. The Sb_6O_{13} electrode exhibited good semiconducting properties applicable to dye-sensitized solar cells (DSSCs): The energy gap was estimated to be 3.05 ± 0.5 eV and the position of conduction band edge was close to those of TiO_2 and ZnO. The DSSC which was assembled using the Sb_6O_{13} photoelectrode and a conventional Ru-dye (N719) exhibited the overall light-electricity efficiency of 0.90 % with the short circuit current (J_{sc}) of 2.41 mA/cm^2 and the open circuit voltage (V_{oc}) of 0.73 V under illumination (AM 1.5, 100 mW cm^{-2}).

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Hybrid solar-cell with inorganic material and water soluble acetylene polymer

이미선, 채강일, 한성환

한양대 화학과

We present a method for preparing water soluble conjugated acetylene based polymer (LM5)-sensitized organic-inorganic hybrid solar cell based on the following device structure ZnO/CdS/LM-polymer/P3HT/Au. The polymer was synthesized in the two ways. First synthesis method is in-situ polymerization and second synthesis method is through direct bulk polymerization route (the polymer was synthesized in the MeOH solvent).It is important to note that conjugated polymers are generally hydrophobic, whereas inorganic compounds are superhydrophilic (water contact angle< 10°). As a result, the hydrophilicity mismatch causes critical problem at the interfacial contact regions .This problem was effectively solved through controlling polymers hydrophilicity. The polymer was modified from hydrophobic to hydrophilic by anion exchange. Therefore we can control the character of interface between the hydrophilic material and hydrophobic material.

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Growth Direction-Controlled Synthesis of Single Crystalline TiO2 Nanowire

박이슬, 이진석

숙명여대 화학과

Nanocrystalline titanium dioxide(TiO2) has been widely studied during the past few years because of its many applications, such as electrodes for electrochemical detection, gas sensors, photocatalysis, dye-sensitization for solar cells, and solar water splitting for hydrogen production. In particular, one-dimensional(1D) TiO2 nanostructure have drawn the attention of worldwide researchers because of their unique characteristics. They have been reported in the published literature in various forms, such as nanotubes, nanowires (NWs), nanowhiskers, nanorods, nanobelts, and nonofibers.TiO2 1D nanostructures have been synthesized by 'wet-chemistry' methods (e.g. electrodeposition, sol-gel electrophoresis, hydrothermal methods, solvothermal methods) and 'dry' methods, such as thermal evaporation and metal-organic chemical vapor deposition. The 'wet-chemistry' processes lack the flexibility to be integrated into semiconductor device fabrication. They also require further heat treatment to improve the crystallinity of the nanostructure, which adds to the complexity of the processes. Here, we synthesized the growth direction-controlled TiO2 NWs, which are , , and , using chemical vapor deposition (CVD) technique as 'dry' method. With changing the growth direction, they are expected to have the distinct crystalline surfaces and energy states, which are exposed to air. Considering the expected physical properties on growth direction-controlled TiO2 NWs, we believe that they can be applied to gas adsorption sensors and photocatalysts with distinguished sensitivity according to growth direction of TiO2 NWs.

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Pentacene derivatives organic photovoltaic cell: simple solution process for film formation

황윤희, 한성환

한양대 화학과

펜타센을 기반으로 하여 합성된 물질을 donor 로 PCBM 을 acceptor 로 사용하여 태양전지에 활용하였다. 모든 물질 층은 용액공정에 의해 만들어졌고, 다양한 방법으로 태양전지를 만들었다. 벌크헤테로정션 태양전지에서는 스프레이나 스핀코팅에 상관없이 비슷한 효율을 얻을 수 있었다. 그러나 bilayer solar cell 은 벌크헤테로정션에 비해 높은 Voc (0.56 V)와 Jsc (1.35mA)를 얻어 0.22%의 효율을 얻었다.

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Hole conducting interfacial in-situ polymerized polythiophene based dye sensitized solar cells

임이슬, Ganesh, 한성환

한양대 화학과

Photoelectrochemical in-situ polymerization enables the formation of uniform polymer layers on the interfacial sites of the Ru-complexes/TiO2 regions. Photopolymerized polythiophene based conducting polymer with intrinsic iodine doping plays an active role as a hole transporting material/layer in DSSCs, reducing the recombination process for enhanced Voc and elevated performance of the solar cell. The influence of iodine doping and polythiophene growth is clearly visualized using X-ray photoelectron spectroscopy and Thermogravimetric analysis, respectively, directly proportional to the performance of the solar cell. The DSSCs with polythiophene layer shows a power conversion efficiency 20% higher compared to one without polythiophene layers

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Chemical Synthesis of Mesoporous ruitle TiO2 nanoparticles films for Liquid and Solid State-dye Sensitized Solar Cells

길병호, 한성환

한양대 화학과

Efficient dye-sensitized solar cells fabricated, using Degusa P25 ¬¬¬¬and sol-gel nanostructures, widely known nanostructures, based on spincoating followed by several annealing procedures are strongly dependent on processing conditions such as spin speed, solvent, surfactant and annealing temperature etc., and faces serious limitations in scalable production. There is need to develop a novel non-complex route from a TiO2 nanostructure point of view, free from these drawbacks, with a competitive solar-to-electrical conversion performance. Here, we show that the low temperature, simple, eco-friendly and economically viable wet chemical method can achieve mesoporous rutile TiO2 nanoparticles films onto fluorine-tin-oxide substrates, a direction for scalable DSSCs, which is free from the use of templates, organic polymers and TiCl4 surface treatment. A photo-conversion efficiency as high as 7% under air mass 1.5 illumination, so far one of the highest conversion efficiencies, is achieved for direct chemically grown TiO2 nanoparticles films without TiCl4 surface treatment in electrolyte system. This low temperature direct synthesis method provides a simple and versatile way to produce scalable mesoporous TiO2 nanoparticles films with the potential to control nanostructures, which can potentially find applications in pigments, sunscreens, paints, ointments, protective coating, photocatalysis, self cleaning glasses, artificial valves, etc.Attempt will also will made to explore results of solid state solar cells devices made from hole carriers P3HT and spiro.

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Unusual energy storage and charge retention in Metal Organic frameworks-71 : influence of phase transformation

이덕연, 윤석준, Ganesh, 한성환

한양대 화학과

Metal-organic frameworks (MOFs)는 지금까지 다양한 분야에서 이용되고 있다. MOFs 의 특징은 secondary building units(SBUs) 구조라는 것과 높은 porosity 를 갖고 있다는 것이다. 이번 포스터에서 우리는 MOF-71 을 capacitor 에 적용한 내용을 기술하였다. 일반적으로 Co 물질은 capacitor 에 적합한것으로 알려져 있다. 이에 우리는 Co 를 metal 로 사용하는 MOF-71 을 이용하여 capacitor 에 적용해 보았다. 다양한 전해질을 이용하여 가장 효과적인 전해질을 찾았으며 비교적 높은 capacitor 값을 얻을수 있었다.

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Development alternative natural dye using Curcumin for Dye-Sensitized Solar Cells

윤석준, 진휘원, Ganesh, 한성환

한양대 화학과

기존의 루테늄 계열의 염료는 제조방법의 복잡성과 경제성, 희귀성 금속의 사용에 따라 염료감응형 태양전지의 생산단가 및 실용화에 장애가 되고 있다. 이에 천연물질로 풍부하게 존재하는 커큐민을 대체염료로 이용하면 이와 같은 문제를 해결할 수 있다. 간단한 산-염기 반응을 통한 염기성 상태의 커큐민을 염료감응형 태양전지에 적용시킴으로서 넓은 파장대의 빛을 흡수, 전지내부 저항, 흡착량 및 결합상수, 전자전이 거동을 통하여 태양전지내에서의 빛흡수 물질로서의 가능성을 연구하였다. 상대적으로 기존 시스템 대비 20%의 빛-전기에너지 전환효율을 낼 수 있지만, 생산단가를 현격히 낮출 수 있기에 염료감응형 태양전지의 실용화에 기여함을 확인하였다.

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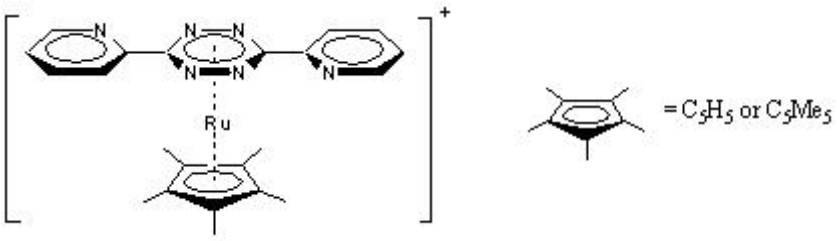
Synthesis and Structural studies of [(3,6-bis(2'-pyridyl)-1,2,4,5-tetrazine)RuCp'][PF6] (Cp' = C5H5, C5Me5)

김윤희, 나영준, 최문근

연세대 화학과

The search for new functional materials is still very active. Among desirable features to achieve, fluorescence as well as the ability to exchange electrons is among the preferred ones, especially when they can be coupled together. The tetrazine ring is the most electron deficient aromatic ring in the CHON chemistry, and in particular in some cases displays a n-π* transition which gives rise to a particular fluorescence with especially long decay times because of the forbidden character of the transition. Its electron deficient character also allows the tetrazine ring to be reversibly reduced by removing one or even two electrons. Some aspects on the fluorescence molecules, molecular materials and polymers based on tetrazines rings, are particularly interesting, and could be enhanced by coupling with other systems such as organometallic systems. Organometallic systems combine also usually a redox property to light absorption, but the introduction of a metal into an organic molecule can also modify the electron density, and therefore change the property of the molecule.The aim of this study is synthesis of (π-tetrazine)RuCp' organometallic complexes for the studies of their photophysical properties.



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Preparation of colloidal precursors from "ball-milling" process in liquid medium for CuInSe2 thin film

정재훈, 최선의, 김승주

아주대 에너지시스템학부

CuInSe2 colloidal precursors have prepared by a mechanochemical synthesis method associated Cu, In and Se metal with different liquid media: (i) toluene, (ii) pyridine in toluene, (iii) ethylenediamine in toluene and (iv) ethylenediamine in dimethylformamide. The phases and the morphologies of resultant precursors were strongly affected by the basicity and polarity of the media. For example, the products from toluene medium were CuInSe2 and Cu1-xInx alloy particles, while the products from the ethylenediamine-containing media exhibited amorphous colloidal aspects. The best suspension stability was observed in the colloids prepared employing the mixture of ethylenediamine and dimethylformamide. CuInSe2 films with the thickness of 1~2 μm were fabricated by deposition of the amorphous colloidal precursor on Mo/glass substrate and successive heating treatments. According to in-situ X-ray diffraction measurement, the CuInSe2 phase started to form above 200oC and showed better crystallinity as temperature increased.

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D-Xylose to Furfural by Dehydration Reactionusing Solid Acid

김은규

아주대 분자과학기술학과

Sulfonic acid (-SO3H) modified mesoporous materials containing HMS, SBA 15 and MCM 41 were synthesized by post-synthesis and co-condensation method. Their catalytic reaction is performed by dehydration reaction of D-xylose to furfural. As a result, good conversion and selectivity was obtained using water as an environmentally friendly solvent. Additionally, increased amounts of sulfuric acid in catalysts resulted in improved conversion of D-xylose. All of the sulfonic acid modified mesoporous materials showed higher selectivity than other solid acids such as γ-Al2O3 and zeolite.

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Fabrication of the high Luminescence Reverse type –I ZnSe core /shell/ shell structure

김성우

아주대 분자과학기술학과

Semiconductor nanocrystals (NCs), and luminescent NCs have attracted considerable interest during the past decade because of their applications in photoelectronic devices and biotechnology. Their opto-electronic properties can be engineered by controlled size, composition and band gap offsets of the core/shell QDs. Core/shell nanoparticles are nanostructures that have core made of a material coated with another material. Core-shell QDs have been classified into three categories, type-I, type-II and reverse type-I according to their band alignments. First, Type-I, such as CdSe/ZnS and InP/ZnSe, contains shell materials with a wider bandgap than the core, which can enhance the quantum yield. Second, Type-II, such as ZnTe/CdSe, ZnSe/CdS, has staggered band alignment between the core and shell and reveals a wide tunable emission wavelength. Finally, reverse type-I structure, such as CdS/HgS, CdTe/InP and ZnSe/CdSe, has a wider band gap than the shell , which suggests the opportunity of an outward-shift of electrons and holes. This results in increased delocalization of the electrons and holes, leading to a red-shift in the absorption and emission.We report the development of cadmium free reverse type-I QDs of ZnSe core/shell/shell.The semiconductor nanocrystals also revealed improved optical properties, with high QY up to about 58% and a tunable emission peak from 430 to 620 nm.

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Three dimensional 5-fold interpenetrated metal-organic framework constructed from 1,4-di(1H-imidazol-5-yl)benzene and cobalt(Ⅱ) ion

박지혜

고려대 화학과

Imidazolates frequently are used for synthesizing metal-organic frameworks(MOFs) such as ZIFs (zeolitic imidazolate frameworks). We have prepared $[Co(p\text{-}dim)_2]\cdot SO_4\cdot H_2O$ (p-dim=1,4-di(1H-imidazol-5-yl)benzene) by a solvothermal reaction of p-dim and Co(Ⅱ) in mixed solvent of H_2O, DMF and triethylamine. X-ray crystallography revealed that the 5-fold interpenetrated 3D framework has Co(Ⅱ) ion coordinated by four nitrogen atoms from p-dim ligands. Sulfates are occupied in pores to maintain charge balance. We will present detailed properties of this compound.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Fluorogenic Assay and Live Cell Imaging of HIV-1 Protease Activity Using FRET-Quenched Quantum Dot-Peptide Complex

최영선, 이정한, 송릿다, *Peter Sommers

*한국파스퇴르연구소 Nano/Bio Chemistry *Cell Biology of Retroviruses Laboratory*

A novel QD-substrate probe for sensing HIV-1 protease activity through the fluorescence recovery of FRET-quenched QD was demonstrated. The peptide sequence-specific fluorogenic property of the QD probe was validated in in vitro assays employing known protease inhibitors and the IC50 values for pepstatin A and the FDA-approved anti HIV-1 drug (Saquinavir) was determined. This probe was also used to detect the protease activity in HIV-1 transfected live cell. Importantly, the effect of SQ effect on protease activity was visualized in HIV-1 infected live HeLa cells. These results provide the potential of this QD probe for the development and implementation of cell-based visual assays for protease-targeted anti-retroviral drug discovery.

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Single Strand vs Ladder: Coordinating Ability of Anions

김은지, 정옥상

부산대 화학과

The reaction of AgX (X^- = NO_2^-, NO_3^-, and ClO_4^-) with new linear spacer, 1,5-bis(isonicotinoyloxy)naphthalene (L), has been carried out. Self-assembly of $AgNO_2$ with L affords ladder-like skeleton consisting of $[Ag_2(NO_2)_2(L)]$ with the trigonal pyramid arrangement around the Ag(I) ion whereas the treatment of $AgNO_3$ or $AgClO_4$ with L yields one-dimensional molecular strand consisting of [Ag(L)](X) with the linear arrangement around the Ag(I) ion. The formation of quite different skeletal structures may be ascribed to the coordinating ability of the anions. That is, nitrite anion acts as a bridged tridentate ligand that connects two silver ions whereas both nitrate and perchlorate anions act as a simple counteranion. Moreover, for the different skeletal structures, anion exchanges were attempted.

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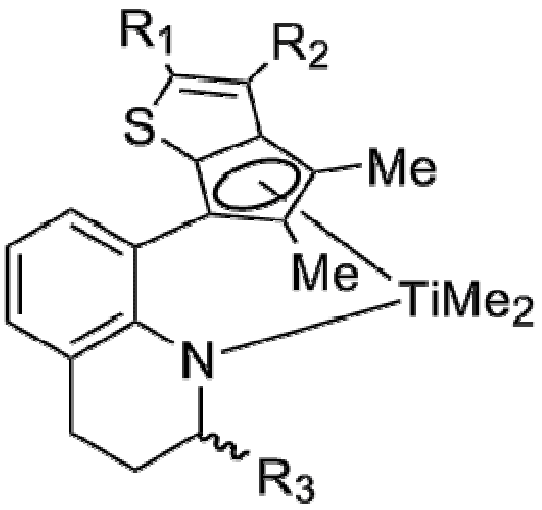
Preparation of half-metallocenes of thiophene-fused and tetrahydroquinoline-linked cyclopentadienyl ligands for ethylene/α-olefin copolymerization

박지혜, 도승현, 이분열

아주대 분자과학기술학과

Directed ortho-lithiation of the lithium carbamates generated from tetrahydroquinoline or tetrahydroquinaldine enables one-step preparation of thiophene-fused and tetrahydroquinoline-linked cyclopentadienes [2-R^1-3-R^2-4,5-dimethyl-6-(2-R^3-2,3,4,5-tetrahydroquinolin-8-yl)-4H-cyclopenta[b]thiophene (R^1, R^2, R^3 = H or methyl)], from which titanium(IV) and zirconium(IV) complexes are prepared. The molecular structures of Me_2Ti-complexes (12, $R^1 = R^2 = Me$, $R^3 = H$; 14, $R^1 = R^2 = R^3 = Me$) and Cl_2Zr-complex (17, $R^1 = R^2 = Me$, $R^3 = H$) are determined by X-ray crystallography. The Me_2Ti-complexes, 14 and 15 ($R^1 = R^3 = Me$, $R^2 = H$) show excellent activities (62 and 54×10^6g/molTi•h) in ethylene/1-octene copolymerization, even when activated with small amount of MAO (Al/Ti = 1000).



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Comparative Study of $[Ru(dmbpy)_2Cl_2]^{0/+}$ and $[Ru(bpy)_2Cl_2]^{0/+}$ Complexes

조명란, 석원경

동국대 화학과

$[Ru(dmbpy)_2Cl_2]^{0/+}$ (dmbpy=4,4'-dimethyl-2,2'-bipyridine) complexes have been synthesized and characterized using spectroscopic and electrochemical techniques. The Ru(II) complex crystallizes in the monoclinic space group $P2_1/a$ with a = 11.3348(8) Å, b = 18.7794(12) Å, c = 12.2102(8) Å and β = 91.2616(19)°, however the Ru(III) complex shows a = 14.1353(8) Å, b = 14.7485(10) Å, c = 15.0360(8) Å and β = 113.5913(13)° in the same space group. The lengths of Ru-Cl bonds decrease while the Ru-N distances increase as the oxidation state of the central ruthenium becomes higher. The structural data of $[Ru(dmbpy)_2Cl_2]^{0/+}$ will be compared with those of $[Ru(bpy)_2Cl_2]^{0/+}$ complexes containing different counter anions.

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Quenching Processes in Light Energy Harvesting in Dendritic Ir(III) Complexes

황아름, *한원식, 조대원, *강상욱

*고려대 신소재화학과 *고려대 소재화학과*

Dendritic Ir(dfppy)$_2$(pic-Cz$_n$) complexes were synthesized, where dfppy, pic, and Cz$_n$ (n = 1, 2, and 3) are 2-(2,4-difluorophenyl)pyridine, picolinate as an ancillary ligand, and 4-phenylcarbazole dendrons, respectively. Selective excitation of the carbazole units in Ir(dfppy))$_2$(pic-Cz$_n$) resulted in fluorescence quenching of excited Cz due to energy transfer to the Ir-complex core. The fluorescence quenching efficiencies of Cz were determined to >90% on the basis of steady-state fluorescence spectra and the decay time constants. The reduced quenching efficiencies of Cz in high-generation dendrimers are probably attributable to the long distance between Cz dendrons and the Ir-complex core. The photoluminescence from the ^{3}MLCT state is enhanced with increasing numbers of Cz dendron units. However, actual enhancement of photoluminescence from the Ir complexes was less than 77% because the ^{3}MLCT emission was quenched by photoinduced electron transfer (PET) from Cz to Ir metal ions. We probed the Cz cation radical species generated by PET in the ^{3}MLCT state by examining the transient absorption.

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Photo-induced Electron Transfer in Heteroleptic Ir(III) Complexes with Light-Harvesting Carbazoles [Ir(dfppy-Cz_n)$_2$(dpq)]

한원식

고려대 소재화학과

We synthesized a heteroleptic Ir(III) complex, Ir(dfppy)$_2$(dpq), and a series of its dendrimer systems, [Ir(dfppy-Cz_n)$_2$(dpq)], where dfppy, dpq and Cz_n (n = 1, 2) are 2-(4,6-difluorophenyl)pyridine, 2,3-bis(2-pyridyl)-qinoxaline, and phenylcarbazole units, respectively, and investigated their photo-physical properties, coupled with photodynamic behavior, to explore possible photo-functionalities of the dendrimers. The complexes revealed a moderately intense, spin-allowed metal-to-ligand charge transfer (^{1}MLCT) band at ~400 nm, and a spin-orbit-coupled triplet-dominated band (^{3}MLCT) at ~500 nm, while the $\pi,\pi*$ transition of the Cz unit occurs at ~300 nm in the case of Ir(dfppy-Cz_n)$_2$(dpq) dendrimers. The phosphorescence of Ir(dfppy-Cz_n)$_2$(dpq) at 650 nm is markedly weaker than that of the parent complex, Ir(dfppy)$_2$(dpq). Transient-spectroscopic studies demonstrated that phosphorescence quenching in Ir(dfppy-Cz_n)$_2$(dpq) occurs by efficient electron transfer from the excited Cz unit to the core ligands, and that the lectron-transfer efficiency decreases with the increase in dendrimer generation associated with an increase in distance between the donor-acceptor pair.

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Graphene sheet and alkyl substituted with alcohol to the synthesis of graphene

진성훈, *조성동

*조선대 화학과 *조선대 화학과*

A new synthetic route for the soluble graphene in organic solvent has been developed from the reaction of graphene oxide with long chain alkylalcohol including dodecylacohol. Grapheneoxide having diverse functional groups of epoxide, alcohol, and carboxylic acid was synthesized from natural graphite powder in inorganic acid solution. The carboxylic acid group among the functional groups was derivatized with long chain alkylalcohols ((CH3(CH2)nOH: n = 7, 11, 14, 18, and 21) to form a strong ester group. The alkylalcohol-derivatized soluble graphene representatives were characterized by UV-vis, IR spectroscopy, and field effect scaning electron micrograph (FE-SEM). This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Synthesis of Photoluminescent Silafluorene Copolymers and Their application for the Detection of Explosives

황민우, 조성동

조선대 화학과

New copolymers containning silafluorenes have been synthesized from the wurtz coupling of dichlorosilafluorene with lithium metal. They were characterized by 1H- and 13C-NMR and their photobehavior were characterized by fluorescence spectroscopy. For possible applications, they used as chemosensor to detect nitroaromatic compounds, such as picric acid (PA), 2,4,6-trinitrotoluene (TNT), 2,4-dinitritoluene (DNT), and nitrobenzene (NB). A linear Stern-Volmer relationship was observed for the analytes. The mechanism of quenching is attributed to electron transfer from the conduction band of copolymers to the LUMO of the analyte. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Syntheses of 1,1-Polysilafluorenes by Catalytic Dehydrocouping for Application as an Expolsive Sensor

김희철, 조성동, 손홍래

조선대 화학과

1,1-Dichlorosilafluorenes and 1,1-dihydrosilafluorenes have been synthesized and their electronic and photonic behaviors were investigated. Polycondensation of 1,1-dichlorosilafluorenes and 1,1-dihydrosilafluorenes were conducted by using an Wultz coupling and dehydrocoupling methods, respectively. To compare the detection efficiencies, 1,1-dihydrosilafluorenes and 1,1-polysilafluorene were served as a chemical sensor. Detection efficiency of 1,1-polysilafluorene was much higher compare to that of 1,1-dihydrosilafluorenes, indicating that the delocalization length for 1,1-polysilafluorene was longer than that for 1,1-dihydrosilafluorenes. These copolymers were characterized by 1H- and 13C-NMR spectroscopies. Photoluminescence efficiencies of these copolymers were measured and compared with their precursor. Photophysical behaviors of these polymers were investigated fluorescence spectroscopy. Further details will be presented. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Synthesis and Characterization of 1,1-Difunctionalgermafluorene and 1,1-Polygermafluorenes for Explosive Sensor Application

엄성용, 조성동

조선대 화학과

Germafluorenes have been synthesized by a route from the stepwise reactions of the 1,2,4,5-tetrabromobenzene, anthracene with tetrachloride germanium in THF at room temperature. The Germafluorenes were characterized by 1H-NMR, 13C-NMR, UV-vis absorption, and photoluminescence spectroscopy. The optical absorption spectra show an absorption edge between 340 nm and 280 nm, while a strong UV-vis photoluminescence between 300 nm and 550 nm is observed. ,1,1-difunctionalgermafluorenes was served as a chemical sensor. Detection of nitroaromatic compound such ad picric acid (PA), TNT, DNT and NB, whose were detected by measuring the quanching photoluminescence of 1,1-difunctionalgermafluorene. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Multilayered Porous Silicon-based Biosensor for the Detection of Biomolecules

양진석, 조성동

조선대 화학과

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. In this paper we investigate the use of a random distribution in the layer thicknesses in order to realize a broadband optical reflector and to such technological motivations, the study of random dielectric multilayers is of interest in the field of one dimensional light localization. This chapter reports on an efficient detection method for the biomolcules simulant based on DBR PSi using laser as incident light sources. Detection of other simulants, streptavidin and Human Ig G, have also been investigated - This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Synthesis and Characterization of Silole/germole-silafluorene/germafluorene Copolymers

조현, 조성동

조선대 화학과

Silole/germole-silafluorene/germafluorene alternating copolymers were synthesized from the reaction of the dilithium salts of tetraphenylsilole dianion or germole with dichlorosilafluorene or dichlorogermafluorene. These copolymers were characterized by 1H- and 13C-NMR spectroscopies. Photoluminescence efficiencies of these copolymers were measured and compared with their precursor. Photophysical behaviors of these polymers were investigated fluorescence spectroscopy. Detection of explosives were investigated for possible applications. Quenching behaviors and other details will be reported. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Detection of CRP Based on Fabrication of anti-CRP Modified DBR Porous Silicon

최태은, 조성동

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 (PS).DBR PS was generated by an electrochemical etching of silicon wafer using two electrode configurations in aqueous ethanolic HF solution using an asymmetric electrode configuration in multiple templates. DBR PS exhibiting unique reflectivity was successfully obtained by an electrochemical etching of silicon wafer using square current waveform. The system was probed with various fragments of an aqueous CRP analyt. This CRP is so named because it is able to affect precipitation of somatic C-polysaccharide of Streptococcus pneumonia. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Solution Synthesis of Alkyl Capped Silicon Nanoparticles of Mg2Si

조보민, 조성동

조선대 화학과

Alkyl-capped silicon nanocrystals have been prepared by the Zintl compound magnesium silicide with bromine. High-resolution transmission electron microscopy confirmed the crystalline nature of the nanoparticles.Energy-dispersive X-ray spectroscopy showed that the nanoparticles are composed of silicon, with no evidence of unreacted chloro. FTIR spectra were consistent with alkylsurfaces. Fluorescence spectroscopy indicated strong ultraviolet-blue photoluminescence, which was attributed to both quantum confinement and surface termination.These nanoparticles displayed long-term stability and no degradation of the photoluminescence was observed for a period of 1 year.- This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Synthesis and Characterization of Silafluorene/germafluorene - silane/germane Alternating Copolymers

이보연, 조성동

조선대 화학과

Silafluorene/germafluorene-silane/germane copolymers were synthesized from the reaction of dilithium salts of silafluoreny and germafluorenyll dianion and dialkyldichlorosilane/germane via Wurtz coupling. These copolymers were characterized by 1H- and 13C-NMR spectroscopy. Photoluminescence of these copolymers were measured by fluorescence spectrometer. Quantum efficiencies of these polymers from the quantum yield of corresponding silafluorene monomer unit were investigated. Comparisons of photobehaviors with other silafluorene copolymer derivatives were achieved. Quenching behavior obtained from the detection of nitroaromatic compounds will be discussed as a chemical sensor. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant number)

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Syntheses and Characterization of Wurtzite CoO, Rocksalt CoO, and Spinel Co3O4 Nanocrystals: Their Interconversion and Tuning of Phase and Morphology

남기민, *서원석, 박준택

*KAIST 화학과 *서강대 화학과*

Cobalt oxides have attracted great interest in their potential applications as catalysts, magnetic data storage devices, lithium-ion battery materials, and solid-state sensors, because of their chemical stability and magnetic properties. However, the formation mechanism and correlation between crystallographic structure and formation kinetics of cobalt oxides have not been clearly explored as of yet. Herein we report a full account of syntheses and characterization of h-CoO and c-CoO nanocrystals with controlled morphologies of hexagonal pyramids, rods, and cubes in a selective manner. The wurtzite and rocksalt phases have been controlled by changing thermal decomposition kinetics of the cobalt precursor, Co(acac)3 (acac = acetylacetonate), in benzylamine. Addition of o-DCB slows down the decomposition rates, and drives the reactions to the thermodynamic control regime. Moreover, through the subsequent air oxidation of both h-CoO and c-CoO nanocrystals, spinel Co3O4 nanocrystals have been produced with retention of the original morphology of CoO. The detailed crystal structures during oxidation reactions have been carefully examined. Finally, the electrochemical properties of h-CoO toward lithium have been investigated for the first time and compared with those of c-CoO and spinel Co3O4 to elucidate their relative electrochemical activities.

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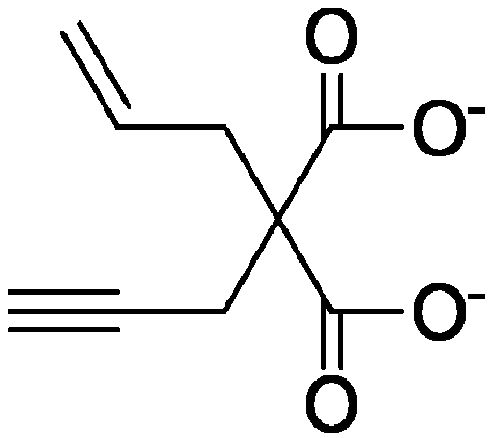
Synthesis of malonatoplatinum(II) complexes and their linkage isomerism dependent on various external condition

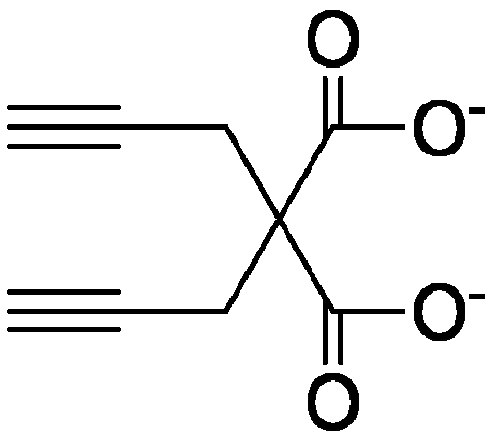
박미영, *이영아

*전북대 나노과학기술학과 *전북대 화학과*

New diamineplatinum(II) complexes, *cis*-Pt(N-N)L_2 (N-N = ammonia (NH_3), ethylenediamine (en), 2,2-dimethyl-1,3-propanediamine (DMPDA), dimethylethylenediamine (DMEDA), tetramethylethylenediamine (TMEDA); L_2 = allylpropagylmalonate (APM), dipropargylmalonate (DPM)), have been sythesized by well-known easy step. The APM and DPM anionic ligands could be possible to chelate with the platinum(II) atom via not only (O,O'), (O,alkene), (O‘, alkyne) but (alkene, alkyne) coordination modes through its two carboxylate groups with the alkene or akyne group, breaking the hard/soft rule. We will observe such coordination modes of malonatoplatinum(II) complexes through FT-IR, NMR, X-ray crystallography.



APM



DPM

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Formation and Properties of New Dithiocarbamate Pt(II) complexes

한아름, 이영아

전북대 화학과

New (dithiocarbamate)platinum(II) complexes $Pt(TC\text{-}X)_2$ (TC-1 = methyl(2-(pyridine-2-yl)ethyl)dithiocarbamate, TC-2 =ethyl(pyridine-2-ylmethyl)dithiocarbamate, TC-3 = bis(pyridine-2-ylmethyl)dithiocarbamate) have been synthesized and characterized by FT-IR, NMR, TGA/DSC, photoluminescence and X-ray crystallography. In crystal structure of $Pt(TC\text{-}1)_2$, platinum(II) atom adopts a typical square planar arrangement with four sulfur atoms of two dithiocarbamate ligands. The four pyridine rings of ligands are situated at the upward and downward from the platinum plane, which is possible coordinating site to other transition metals. $Pt(TC\text{-}X)_2$ series is a novel bidentate or tetradentate metallo-ligand to make various macromolecules. Interestingly, $Pt(TC\text{-}1)_2$ and $Pt(TC\text{-}3)_2$ show orange luminescence (λ_{em} = 567.5 nm for $Pt(TC\text{-}1)_2$, 564 nm for $Pt(TC\text{-}3)_2$) at room temperature in solid state, but $Pt(TC\text{-}2)_2$ didn't show any luminescent properties at room temperature. The fluorescence intensity enhancement was observed at 77K.

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Synthesis and Physical Properties of New Au(I) Complexes with Dithiocarbamate Ligands

한세미, 이영아

전북대 화학과

A new series of complexes, $[Au_2(P\text{-}P)(TC\text{-}2)]X$ and $Au_2(P\text{-}P)(TC\text{-}2)_2$ (P-P = dppm, dppe, dppp ; TC-2 = ethyl(pyridin-4-ylmethyl)carbamodithioate ; X = CF_3CO_2, BF_4, PF_6), were synthesized. These complexes were characterized by FT-IR, NMR, photoluminescence and X-ray crystallography. In $Au_2(dppe)(TC\text{-}2)_2$ crystal structure, TC-2 and phosphine ligands bridged two Au(Ⅰ) ions, each having a transoid coordination geometry and a Au…Au intramolecular distance of 3.0169 (2) Å. The $Au_2(P\text{-}P)(TC\text{-}2)_2$ complexes show no luminescence. otherwise $[Au_2(P\text{-}P)(TC\text{-}2)](CF_3CO_2)_2$ complexes show bright luminescence at λem = 535 nm. The emission properties of Au complexes have relation to alkyl chain length of phosphine ligands. $[Au_2(P\text{-}P)(TC\text{-}2)]X$ luminescent property depend on X exchange.

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Synthesis and Characterization of Silver Nanoparticles Facilitated by Inclusion Complex of β–Cyclodextrin with Hydrosilane

우희권

전남대 화학과

Silver nanoparticles are prepared in a controlled aqueous medium including an inclusion complex, formed between β-cyclodextrin (β-CD) and phenylsilane (PS). The inclusion complex, β-CD/PS stabilizes the Ag nanoparticles preventing agglomeration and provides self-assembling environment for forming composite structure around Ag nanoparticles. The reduction of silver (Ag+) salts to silver (Ag0) nanoparticles is facilitated by phenylsilanes tightly capped in the β-CD. The nanoparticles were characterized using XRD, TEM, FE-SEM, and solid-state UV-vis analytical techniques. TEM and FE-SEM data show that the size of silver nanoparticles is observed to be about 10 nm. XRD patterns indicates the presence of fcc silver.

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Synthesis and Characterization of Germane/Stannane-capped Polysiloles for Fabrication of Luminescent OLED

우희권

전남대 화학과

Siloles (i.e., silacyclopentadienes) having a low reduction potential and a low-lying LUMO, have received great attention and can be used for electron-transporting materials in OLED devices. Polysilole could exhibit different luminescent behavior from that of monomeric siloles. We recently reported the synthesis of polysilole having hydrogen end groups by the homogeneous dehydrocoupling of 1,1-dihydrotetraphenylsilole using an inorganic hydride (Red-Al). The germane/stannane-ended polysiloles have been prepared by the catalytic dehydrocoupling of 1,1-dihydrotetraphenylsilole in the presence of Red-Al, followed by capping with diphenylchlorostannane or dimethylchlorogermane. The germane/stannane-ended polysiloles can be easily transformed to the other group-ended polysiloles by simple chemical reactions. The nano size of functional polysiloles emit green light at 520 nm and are electroluminescent at 520nm like hydrogen-ended polysilole.

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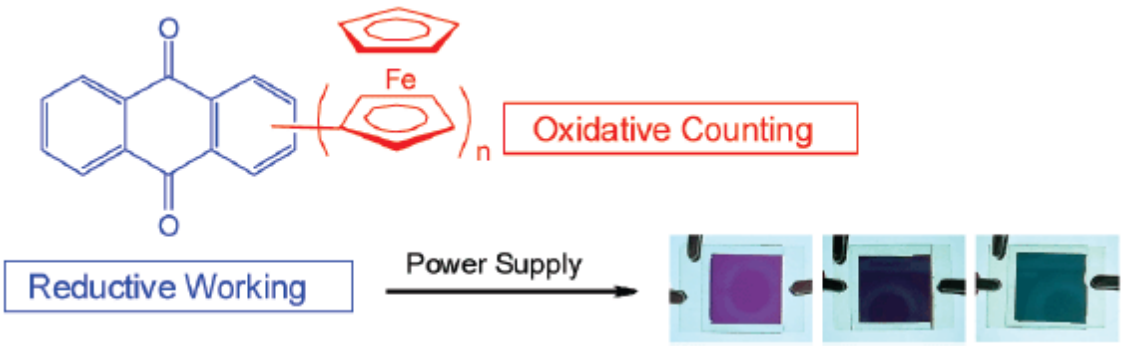
Designed Synthesis of Ferrocenylanthraquinones and Their Bifunctional Electrochromic Properties

walidsharmoukh, 손성욱

성균관대 화학과

New bifunctional electrochromic systems were developed by combination of reductive anthraquinone with oxidative ferrocene redox systems.The resultant ferrocenylanthraquinones demonstrated enhanced stability in electrochromic performance through the concomitant reductive electrochromism and oxidative counting action. The displayed colors were dependent on the position of the ferrocenyl group.



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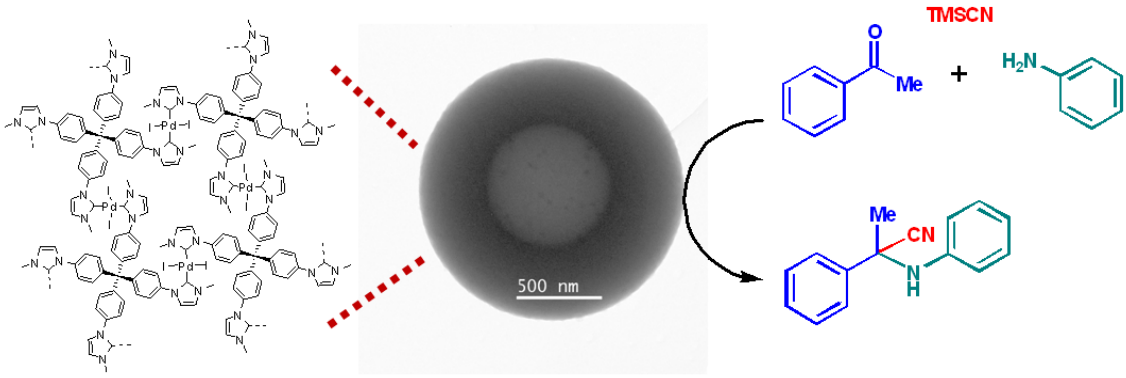
Organometallic Hollow Spheres Bearing Bis(N-Heterocyclic Carbene)-Palladium Species: Catalytic Application in Three-Component Strecker Reactions

양혜윤, 최재원, 손성욱

성균관대 화학과

Organometallic hollw spheres bearing $(NHC)_2Pd$ species were prepared for the first time by a template-free route using tetraimidazolium building blocks and palladium acetate. Their physical structure and properties were characterized by SEM, TEM, microtoming experiments, and TGA, and their chemical composition by EDS, solid-phase 13C NMR spectroscopy and EA. The ofganometallic hollow psheres demonstrate excellent activities as heterogeneous catalysts in one-pot three-component Strecher reactions of ketones.



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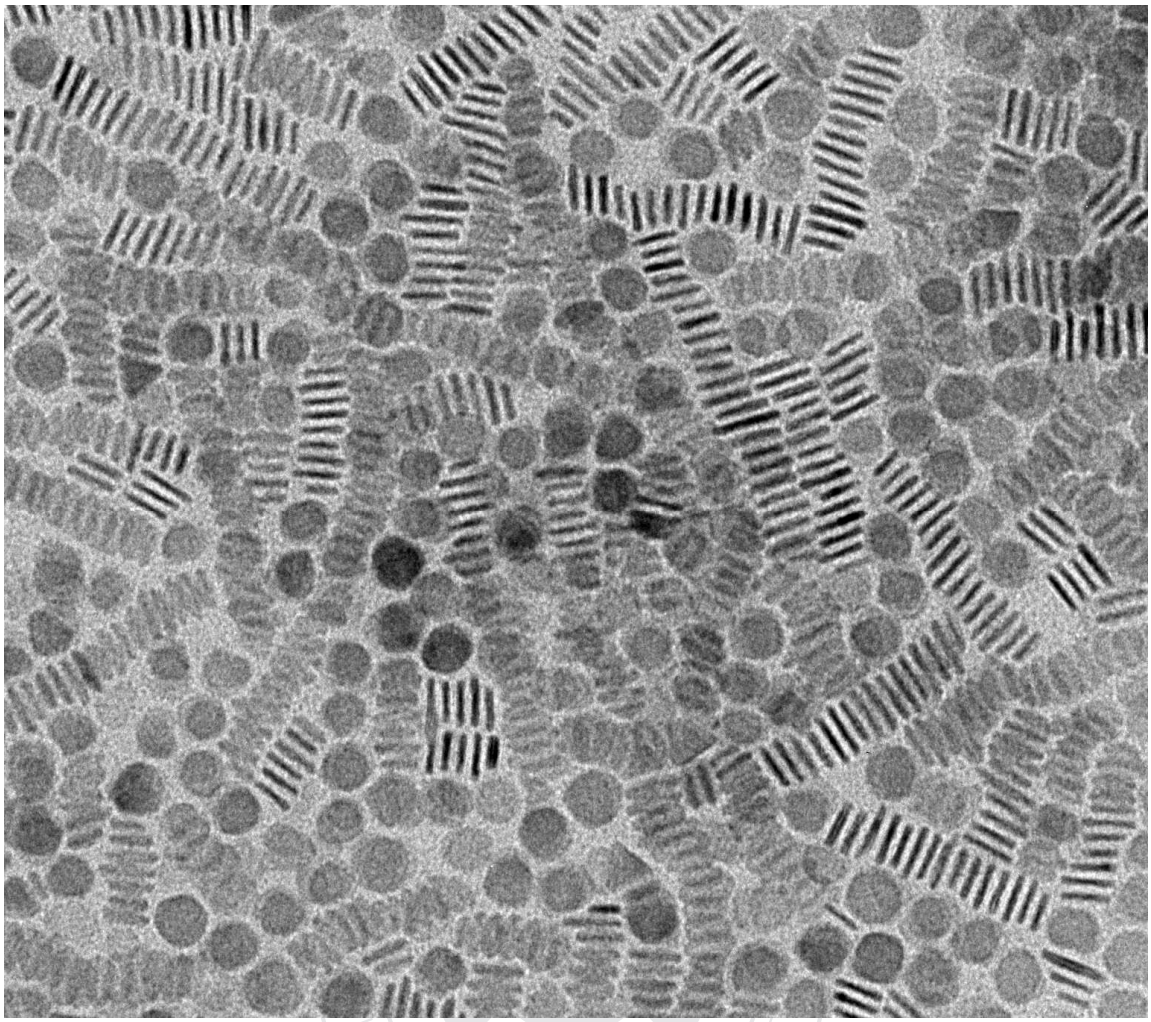
Colloidal Synthesis of Cubic-Phase Copper Selenide Nanodiscs and Their Optoelectronic Properties

최재원, 양혜윤, 손성욱

성균관대 화학과

high-quality copper selenide nanodiscswith a 2.6 nm thickness were prepared using imidazoline-2-selenone as a new selenium precursor. The phase of prepared nanomaterials was characterized to be cubic Cu2-XSe by HR-TEM, XRPD, EDX and XPS and promising optoelectric properties were observed.We believe that the copper selenide discs in this study can be applied to development of the n/p semiconductor type solar cell devices via a solutionbased approach.

THE KOREAN CHEMICAL SOCIETY



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Construction of Porphyrin-Viologen Dyads through Covalent and Non-covalent Linkages

김민경, 김빛나라, 김희준

금오공과대 응용화학과

Multicomponent donor-acceptor systems and their photo-induced energy or electron transfer processes have been received great attention with the goals of understanding the primary processes in natural photosynthesis and of designing photochemical molecular devices for energy conversion. Porphyrins are popularly employed as suitable photoactive components in multicomponent systems.Porphyrin and metalloporphyrins have been used as electron donors and methylviologen (N,N-dimethyl-4,4-bipyridinium, MV^{2+}) is a common electron acceptor in studies of electron transfer reactions. Thus, we have been interested in construction of porphyrin-viologen dyads through covalent and non-covalent linkages

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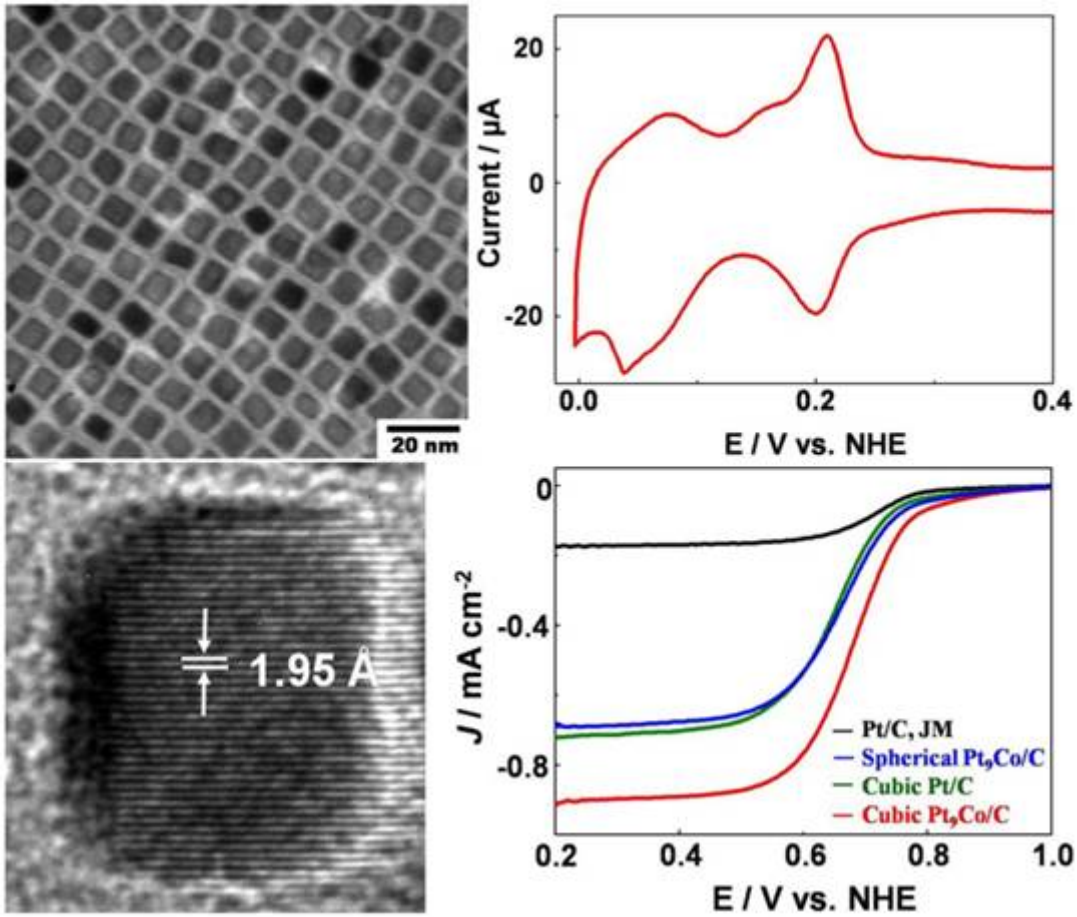
Synthesis and Characterization of Pt_9Co Nanocubes with High Activity for Oxygen Reduction

최상일

KAIST 화학과

Pt nanoparticles are the most efficient catalysts for the oxygen reduction reaction (ORR) at the cathode in a polymer electrolyte membrane fuel cell (PEMFC). Although it has a high catalytic activity, Pt is expensive due to its limited supply. In this regard, improving the activity of Pt, thereby decreasing the amount needed in electro-catalysis, has been extensively investigated. Important strategies for developing highly active Pt catalysts have included the control of the surface arrangements of the Pt particles and the use of Pt-based bimetallic particles in place of pure Pt as the electro-catalyst. Previous studies on ORR in acidic media have shown that Pt {100} planes are more active than are Pt {111}, and thus the catalytic activity of Pt nanocubes is much higher than that of polyhedral and truncated cubic Pt nanoparticles. In addition, recent reports reveal that the ORR activities of Pt-M (M = Co, Ni, Fe, Cr, Cu, V, and Pd) alloys are superior to those of pure Pt nanocrystals. The synthesis of Pt alloy nanocatalysts with controlled morphologies is, therefore, one of the most critical issues for enhancement of their catalytic activities.4 We herein report on the synthesis of monodisperse, highly crystalline Pt_9Co nanocubes with significantly enhanced electrocatalytic activity toward ORR. The shape of the Pt_9Co nanoparticles was controlled by oleylamine/oleic acid stabilizers and the molar ratio of Pt and Co precursors.



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Characterization of optical properties of SiO_2-deposited ITO film

김정수, *최식영, *임우택, 박미영, **김혜영

*안동대 화학과 *안동대 응용화학과 **안동대 화학교육과*

Tin-doped Indium Oxide (ITO) thin films in polyethylene terephthalate (PET) were prepared by Roll-to-Roll sputter system with both targets of ITO and SiO_2. RF power and DC power were used to deposit for $SiO_2$and ITO, respectively. The deposition of SiO_2 and ITO was performed with RF power of 400 W, Ar gas of 50 sccm, and O_2 gas of 0 sccm and DC power of 600 W, Ar gas of 50 sccm, O_2 gas of 0.2 sccm, and winding speed of 0.64 m/min, respectively. Their characteristic properties were analyzed by spectrophotometer and 4-point probe. ITO thin film without SiO2 layer had chromaticity of 2.87, resistivity of 400 ohm/sq, and transmittance of 88% and SiO_2-doped ITO thin film with chromaticity of 2.01, resistivity of 709 ohm/sq, and transmittance of more than 90% were obtained. As a result, SiO_2 was coated on PET before deposition of ITO, their chromaticity (b*) and transmittance were better than previous results of ITO films. It showed that coating of SiO_2 induced a rising chromaticity (b*) and transmittance. If the thickness of SiO_2 is controled, sheet resistance value of ITO film will be expected to be better for touch screen.

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Synthesis and Characterization of Biofunctionalized Tetraphenylsilole and Its Application as a Biosensor

이보연, 손홍래

조선대 화학과

Biofunctionalized tetraphenylsilole was synthesized from the reaction of aminopropylmethylsilole with biotin and characterized by 1H- and 13C-NMR spectroscopy. Quantum yield of biofunctionalized tetraphenylsilole was measured by fluorescence spectrometer. The aggregation of behavior of this molecule in colloid was investigated by the measurement of photoluminescence. Detection of biomolecules such as streptavidin and avidin in colloid was achieved by the measurement of quenching photoluminescence. Quenching photoluminescence of biofunctionalized tetraphenylsilole was result in an electron transfer from silole to biomolecule analytes. Further details on photobehaviors of biofunctionalized tetraphenylsilole will be discussed. This research was supported by WISE center of Chosun University in GwangJu, Chonnam.

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Supramolecular Architecture of 7-azaindole based Ag(I) Complexes

강영진, *김진호, **박기민, *이은지, *정나래

*강원대 과학교육과 *강원대 화학과 **경상대 화학과*

Nitrogen heterocycles are extensively used as ligands in coordination chemistry, and the search of new ligands for novel self-assembled metallosupramolecular architectures remains of great interest. Among the nitrogen heterocycles, especially, nitrogen-donor chelated organic ligands based on 7-azaindole have recently attracted considerable interest because of their applications in organic light-emitting diodes (OLEDs), coordination chemistry of main groups and/or transition metals, and their functionalities of potential building blocks for supramolecular nanoengineering. Interestingly, the coordination modes to group 10 or group 11 metal ions vary according to ligand used and the position of 7-azaindole unit in benzene ring. We present here a new synthesis of 1,4-bis(7-azaindolyl)benzene and its silver complexes.

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Alkyl-functionalized Organic Sensitizers for Efficient Dye-Sensitized Solar Cells(DSSCs)

강영진, *김진호, *이은지, *정나래

*강원대 과학교육과 *강원대 화학과*

Two organic dyes, 2-Cyano-3-[5´´-{N,N-bis(9,9-diphenyl-9H-carbazol-3-yl)phenyl}-[2,2´,5´,2´´]terthiophenyl-5-yl]acrylic acid(CTTA) and 2-Cyano-3-[5´´´-{N,N-bis(9,9-diphenyl-9H-carbazol-3-yl)phenyl}-3´,3´´,3´´´,4-tetra-n-hexyl-[2,2´,5´,2´´,5´´,2´´´]-quarter thiophenyl-5-yl]acrylic acid(CTQA), containing diphenylcarbazolyamine and hexylthiophene groups are designed and synthesized. Nanocrystalline TiO2 dye-sensitized solar cells were fabricated using these dyes. Under standard global AM 1.5 solar condition, the CTQA sensitized solar cell gave a short circuit photocurrent density of 16.04 mA/cm2, open circuit voltage of 0.65V, and fill factor of 0.71, corresponding to an overall conversion efficiency η of 7.43 %.

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CARBOSILANE DENDRIMER AND HYPERBRANCHED POLYCARBOSILANE

남은희, 박경헌, 이선정, 신대식, 김정균

동아대 화학과

Carbosilane dendrimers with phenylethynyl, anthracenyl, benzoxazoyl, cholesteryl and perfluorinated groups on the periphery were prepared. The core molecule siloxane tetramer with vinyl groups is branched to produce higher generations of carbosilane dendrimers by the iterative hydrosilation and alkynylation cycles. Hyperbranched polycarbosilane with cholesteryl and perfluorinated groups on the chain were prepared. The unreacted allyl groups on hyperbranched polymer are introduced to bigger molecule by dendritic growing methods.Key words: Dendrimer, Silane, Hyperbranched polymer, Encapsulation.

THE KOREAN CHEMICAL SOCIETY

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Synthesis and characterization of SubPc-Porphyrin-SubPc triad linked by axial coordination

노수민, 박수영, 김희준

금오공과대 응용화학과

Porphyrins and subphthalocyanines (SubPc) are attractive components suited for devising integrated, multicomponent model systems to transmit and process solar energy. Therefore, the construction of novel molecular arrays consisting of porphyrins and subphthalocyanines is an appealing target. However, porphyrin-subphthalocyanine complexes through axial coordination of metalloporphyrins are very rare. We will present the synthesis and characterization of SubPc-Porphyrin-SubPc triad linked by axial coordination in detail.

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Modification of silica surface with various saline coupling agents to control property of silica

이규민, *유중환

*고려대 화공생명공학과 *한국세라믹기술원 에코복합소재센터*

Silica surface was modified with various silane coupling agents to change property of silica. Various functional groups containing sulfur chain or alkyl chain were used to modify silica surface. FT-IR, TGA and 29Si CP/MAS NMR confirm modification of silica surface with silane coupling agent chemically or physically. Silane coupling agent on the silica surface is analyzed by infrared spectra peaks at 2962, 2927, 2855 cm-1 due to stretching vibration modes of the C-H bonds. The chemical modification of silica leads to chemical T and Q peak shift in NMR spectra. After modification, amount of physisorbed water on the silica is decreased, while organic amount on the silica is increased. From SEM analysis, unmodified silica is agglomerate in the rubber, however, modified silica is well dispersed in the rubber composite because filler-filler interaction was reduced by modification.

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Multifunctional Heterometallic Lanthanide MOFs: Exchange of Metal Ions and Structural Transformations

이우람, 홍창섭

고려대 화학과

Three-dimensional heterometallic frameworks of $(H_3O)[LnZn(TPO)_2](DMF)(H_2O)$ (Ln = Eu, Tb) were synthesized by a solvothermal reaction of lanthanide nitrate and zinc nitrate in DMF at 100°C for 48 h. Single crystal X-ray diffraction shows that they crystallize in the P-1 space group. The structures of both complexes contain heterometallic SBU formed by Ln and Zn ions. 1 shows selective sorption property for CO_2 at 273 K. When 1 and 2 were immersed in europium nitrate and terbium nitrate in DMF for 60 h at 100°C, each metal ion was exchanged by Eu(III) and Tb(III) ions as confirmed by ICP-AES and luminescence properties. Single crystal X-ray structures, sorption and luminescent properties of the title compounds will be presented in detail.

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The Chemical Reactivity of 4-BBDT on Edge and Basal Plane of Graphene and Its Doping Effect

임현섭

포항공과대 화학과

The site-dependent and spontaneous functionalization of 4-bromobenzene diazonium tetraflouroborate (4-BBDT) and its doping effect on a mechanically exfoliated graphene (MEG) have been investigated. The spatially-resolved Raman spectra obtained from both edge and basal region of MEG have revealed that 4-BBDT molecules are non-covalently functionalized on the basal region of MEG where structural defect is almost absent, while they are covalently bonded to the edge of MEG. The chemical doping effect induced by the non-covalently functionalized 4-BBDT molecules on the basal plane region of MEG has been successfully elucidated by Raman spectroscopy. The position of Fermi level of an original MEG and its systematic change upon the change of doping level have been clarified from G band changes, while the doping type has been determined by 2D band changes. The successful establishment of such a correlation between chemical doping effect and Raman spectral feature change is highly beneficial for the fundamental studies about the charge transfer phenomena of graphene as well as for the potential applications, such as electronic devices, hybridized composite structures, etc.ReferenceLim, H.; Lee, J.; Shin, H.-J.; Shin, H. S.*; Choi, H. C.* Langmuir 2010, 26, 12278.

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Solution phase fluorination on single walled carbon nanotubes

박지은

포항공과대 화학과

Incorporation of heteroatomic moieties into the backbone of single walled carbon nanotubes (SWNTs) is a direct gateway toward the versatile passivation of SWNTs with various active functional groups. Among many candidates, fluorine is of special interest not only because fluorine has been known as a good leaving group which enables further substitution reactions, but more importantly because its strong electronegativity allows facile tuning of the doping level of semiconducting SWNTs. Until now, the fluorination of SWNTs has been available only by gas phase reaction in which toxic fluorine gas should be involved. More seriously, the gas phase fluorination requires long reaction times at high temperature. In this presentation, we will discuss about a newly developed fluorination of SWNTs in solution phase at room temperature. We confirmed the successful fluorination of SWNTs by X-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (IR). The detail proposed mechanism of the fluorination will be also discussed.

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Formation of Germanium Selenide (GeSe) comb structures by simple vapor deposition and their optoelectronic properties

송현재, *최희철

*포항공과대 화학 *포항공과대 화학과*

Chalcogenides represented by II-VI and IV-VI compounds have been widely investigated to exploit their unique optical and electrical properties into UV-visible-infrared optics, photovoltaic cells and thermoelectric devices applications. Up to date, most of chalcogenides have been concentrated on II-VI compounds due to their feasible synthetic methods and excellent quantum size effects. Germanium selenides, having a narrow band gap energy, have been less highlighted in spite of its wide usages as memory cells and glass forming materials. It seems to be due to the lack of facile synthetic routes to low dimensional single crystalline structures, while lead chalcogenides displaying the thermoelectric properties and germanium telluride showing phase-change memory properties have been demonstrated, recently.Here we report the facile synthetic method for single crystalline germanium monoselenide (GeSe) comb structures via atmospheric pressure vaporation-condensation-recrystallization (VCR) process using single precursor, bulk GeSe powder. The synthesized GeSe combs display p-type semiconducting transport property as well as photo-switching property. Based on morphological investigations, growth mechanisms are proposed.

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DBR, Rugate Porous Silicon by Asymmetric Electrode Configuration using square form for Biosensor Application

조성동

조선대 화학과

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. Films with pore sizes in the range of a few nanometers are used as size-exclusion matrices to perform an on-chip determination of macromolecule dimensions. This reflective wavelength can be controlled by tuning of etching time and can appear anywhere in the visible range depending on the square and sine waveform. This might be a demonstration for the fabrication of specific reflectors or filters in full color.Optical reflectivity spectra of the thin porous Si films display distinctive shifts in the Multi layer in regions of the film where the pore dimensions are larger then a critical size, interpreted to be the characteristic for Biosensor Application.

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n-Type Porous Silicon of Photoluminescence Efficiency by Controlling of an Current Densities and Applied Etching Time

조성동

조선대 화학과

Porous silicon films were prepared by an electrochemical etch of n-type silicon (phosphorous doped, orientation) in an ethanolic solution of hydrofluoric acid. Photoluminescence of porous silicon was investigated by controlling of an etching time and applied current densities from 50 sec. to 900 sec. and from 50 mA/cm2 to 800 mA/cm2, respectively. Photoluminescence efficiencies of prepared porous silicon samples were measured at given applied current density. As etching time increased, the photoluminescence efficiency of porous silicon prepared increased. However, this photoluminescence efficiency start to decrease, after it reach to the maximum efficiency with further etching time. Porous silicon sample shown the best photoluminescence efficiency was prepared with 200 mA/cm2 of applied current density and with 300 sec of etching time.

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Multi –Encoded Rugate of Polymer Replicas Templated from a Nanostructure of Oxidized Porous Silicon

조성동

조선대 화학과

Rugate structure result in a mirror with high reflectivity in a specific narrow spectral region and are prepared by applying a computer-generated pseudo-sinusoidal current waveform. Strategies to encode multiple rugate structures have been investigated. Multiple rugate structures can be etched on a silicon wafer and placed in the same physical location, showing that many sharp spectral lines can be obtained in the optical reflectivity spectrum. Etching is carried out in a Teflon cell by using a two-electrode configuration with a Pt mesh counter electrode. Rugate PSi films can be lifted off from the silicon substrate to obtain a free-standing rugate PSi films. For many applications, free-standing rugate PSi is limited by its chemical and mechanical stability. The photonic polymer replicas showing a desired reflectivity by casting of polymer solution onto a porous silicon dioxide multilayer have been prepared. The photonic polymer replicas are robust in ambient condition and exhibit an excellent reflectivity in their reflective spectra. The photonic band gaps of replicas are narrower than that of typical semiconductor quantum dots. The means for the construction of complex photonic structures with polymers have been provide.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

DFT study of collective rearrangements of atoms in tubular boron cluster I

장효원

순천대 화학과

The information about the thermal stabilities of boron clusters is valuable for any application of boron nanostructures to electronic devices aimed to operate at high temperatures utilizing their semiconducting properties. It is worthwhile to consider collective motions of atoms maintaining tubular shapes because they could serve as building blocks for longer nanowires.In this work, we study the energetics during such rearrangement reactions of tubular clusters with popular density functional theory (DFT) method of quantum chemistry.By calculating the reaction paths and the activation energies between stable conformations, we could analyze the structural integrity, and subsequently their accompanying electonic properties.

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Prototropic Equilibrium Dynamics of Excited-State 6-Hydroxyquinoline in Faujasite Zeolitic Nanocavities

박선영, *유현웅, **박지호, 장두전

*서울대 화학부 *한국표준과학연구원 전략기술연구부 **한국방송통신대 환경보건학과*

The excited-state proton transfer and geminate recombination of 6-hydroxyquinoline (6HQ) encapsulated in microporous catalytic faujasite zeolites of Na^+-exchanged X (NaX) and Y (NaY) have been explored by measuring steady-state and picosecond time-resolved spectra. The pathways as well as the rate constants of the proton transfer of excited 6HQ are determined by the microscopic environment of zeolitic hosts surrounding the guest molecules. The excited-state tautimerization of 6HQ in zeolitic nanocavities is initiated by the deprotonation of the enolic group to form an anionic intermediate and completed by the subsequent protonation of the imino group to form a zwitterionic tautomer. Geminate recombination occurs to compete with proton transfer at each tautomerization step of excited-state 6HQ because of the confined environment of dehydrated zeolitic nanocavities. Consequently, excited-state equilibria among three prototropic species of 6HQ are established in microporous catalytic faujasite zeolites. Differences of kinetic properties between 6HQ-intercalated NaX and NaY are attributed to dissimilarities in acidity/basicity of NaX and NaY.

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Photoinduced Double Proton Transfer Dynamics of Model DNA Base Pairs: 7-Hydroxyquinoline Dimers

임형택, 박선영, 장두전

서울대 화학부

The excited-state double proton transfer of model DNA base pairs, 7-hydroxyquinoline dimers, in benzene has been investigated using picosecond time-resolved fluorescence spectroscopy. Upon excitation, whereas singly hydrogen-bonded noncyclic dimers do not go through tautomerization within the relaxation time of 1400 ps, doubly hydrogen-bonded cyclic dimers undergo excited-state double proton transfer on the time scale of 25 ps to form tautomeric dimers, which subsequently undergo a conformational change in 180 ps to produce singly hydrogen-bonded tautomers. The rate constant of the double proton transfer reaction is temperature-independent with showing a large kinetic isotope effect of 5.2, suggesting that the rate is governed mostly by tunneling.

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Room-Temperature Ultraviolet Emission of Arrayed ZnO Nanowires on Zn Foil

김종엽, 정혁, 장두전

서울대 화학부

Well-ordered nanowires of the hexagonal wurtzite ZnO having an average diameter of 80 nm, a typical length of 12 μm, and a mean packing density of 7.5 nanowires μm^{-2} have been directly grown on Zn foil in a preferred [0001] direction by a hydrothermal process and employed for room-temperature ultraviolet nanolasers. The relative texture coefficient of the (002) diffraction peak over the (100) diffraction peak was measured to be 0.91, suggesting that ZnO nanowires were grown along the [0001] direction following the crystal orientation of the c-axis. A suitable concentration of $Zn(OH)_4^{2-}$ ions played a key role for the growth of 1D ZnO nanowire arrays on Zn foil. The lasing action of arrayed ZnO nanowires has been observed at ultraviolet wavelengths varying from 370 to 400 nm with an emission line width of 0.08 nm. The excitation irradiance dependent lasing action of well-ordered ZnO nanowire arrays on Zn foil has been found to have threshold irradiance of 25 kW cm^{-2}, which is much lower than the value (70 kW cm^{-2}) reported for ZnO nanorod arrays on Si wafer. Photoluminescence decays biexponentially: the fast component is attributed to freeexciton decay, and the slow one is to bound-exciton decay. The amplitude of the fast component increases whereas its lifetime decreases with the increment of the excitation irradiance, suggesting that ZnO nanowire arrays undergo a change in the lasing mechanism from exciton-exciton scattering to electron-hole plasma recombination.

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Hollow Pt/Ag Nanocomposites: Galvanic Fabrication and Their Enhanced Catalytic Properties

김미란, 이동기, 장두전

서울대 화학부

Pt/Ag composite nanospheres, which show highly enhanced catalytic properties, have beenprepared through a galvanic replacement reaction of silver nanoparticles dispersed inPt^{n+}-added water. Pt^{n+}, prepared in advance by the partial reduction of Pt^{4+} with weak reducing agents, is readily reduced galvanically to form porous Pt shells, and concomitantly produced Ag^{+} diffusesout to produce hollow Pt/Ag nanocomposites finally. The residual silver has been furthereliminated from the composites with 0.5 M HNO_3(aq) to produce hollow Pt nanospheres. HollowPt/Ag composite nanostructures have been found to catalyze the degradation of rhodamine Befficiently in the presence of KBH_4, although their catalytic performances depend highly on the15 metals, sizes, and shapes of the nanostructures.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of Highly Luminescent InP@ZnSe Nanoparticles

김미란, 김형배, 이성훈, 장두전

서울대 화학부

InP quantum dots of 3 nm in diameter have been prepared using a dehalosilylation reaction and passivated with ZnSe to enhance photoluminescence by 6.8 times. Core–shell InP@ZnSe quantum dots dispersed in n-hexane have then been investigated using time-resolved spectroscopy to understand their photoluminescence dynamics. The observed decay times of 0.1, 7, and 1100 ns have been attributed to the relaxation times of electrons in the conduction band, trap sites, and surface states. The surface-state luminescence of core–shell InP@ZnSe quantum dots having the maximum at 760 nm has been distinguished spectrally and dynamically from their band-edge emission having the maximum at 620 nm or from their trap-site emission having the maximum at 660 nm.

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Photodissociation spectroscopy of aniline-water-benzen cluster cation

MD.ALAUDDIN

경희대 화학과

The infrared photodissociation spectroscopy of aniline-water-benzene cluster cation (AWB+) in NH and OH stretching region has been investigated. It has been found that an infrared photon can decompose the cluster cation AWB+ into fragments in two different reaction paths: AWB+ + hν→ AW+ +B and AB+ + W. We also observed the vibrational mode dependence of the branching ratio of the infrared photodissociation reaction of the ternary hydrogen bond cluster.

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Deuteration effect on the solvent-assisted conformational isomerization of 3-aminophenol

김민호, 손운용, *김상수, *강혁, *박영동

*아주대 에너지시스템학부 *아주대 화학과*

3-aminophenol (3AP) has two conformers, *cis* and *trans*, depending on relative orientation of the OH group towards the NH_2 group, of which the *trans* conformer is the more stable one. When 3AP makes a cluster with a solvent, the binding energy of the cluster is available as excess energy to overcome the isomerization barrier between *cis* and *trans* conformers, thus solvent-assisted conformation isomerization (SACI) occurs. The SACI drives the population of the less stable *cis* conformer to the more stable *trans* conformer. In previous experiments we attached several solvent molecules to 3AP to tune the binding energy, and observed the SACI yield as a function of the binding energy in order to determine the isomerization barrier height. In the current experiment, we deuterated the hydroxyl group to tune the barrier height and observed the SACI at different barrier height.

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Correlation of the Solvolyses of Diphenyl, Bis(2,4-Dichlorophenyl) and Bis(4-Chlorophenyl) Phosphorochloridate

고한중

전주교육대 과학교육과

Specific rates of solvolysis of diphenyl(1) and bis(2,4-dichlorophenyl)(3) phosphorochloridate (chlorophosphate) have been determined by a conductivity technique. The available specific rates together with those determined earlier for bis(4-chlorophenyl) phosphorochloridate(2) have been analyzed in terms of the extended (two-term) Grunwald-Winstein equation. It is found that rather poor overall correlations found earlier for 1 and 2 and now for 3 are considerably improved when data points for 2,2,2-trifluoroethanol-ethanol and acetone-water mixtures are excluded. The large sensitivities toward changes in solvent nucleophilicity are consistent with a bimolecular process. The variation in nucleophilicity of the acetone-water mixtures for attack at carbon or at phosphorus is discussed.

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Theoretical Studies on the Alkali Metal Cation Effects for theReactions of Phenyl Aryl Chlorophosphates with pyridines in the GasPhase and in Aqueous Solution

한인숙, 김창곤, 김찬경, 이해황, *이본수

*인하대 화학과 *인하대 총장실*

The Effects of Alkali-Metal Cation, X^+ (=Li^+, Na^+, K^+), for the substitution reactions of phenyl arylchlorophosphates, $C_6H_5OP(=O)(Cl)OC_6H_5$, with pyridines have been studied theoretically in the gasphase and in aqueous solution. All the reactions were found to proceed via a concerted mechanism with the nucleophile(pyridine) and leaving group (Cl) occupying apical sites at the transition states (TS). On the contrary, for the reactions without X^+, the TSs via a concerted process or any stable intermediates could not be located as stationary point species on the reaction coordinates in the gas phase. This indicates that the effects of X^+ play a considerably important role. All the stationary point species have been fully optimized and characterized by frequency calculations at RHF level with 6-31+G(d) and at B3LYP level with 6-311+G(d) and 6-311+G(2d,p) basis sets.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Assembly of the multi-segmented, Se-Te-Se nanorods

박미선, 김진권, 김상호

공주대 화학과

The side-by-side assembly of nanorods are interesting phenomena in nanoscience. Typically, this assembly is well understood by the energetic effect originated from the parallel interaction between nanorods and the entropic effect by minimizing the excluded volume of solvent during evaporation. The basic understanding of side-by-side assembly in nanorod system is further explored in the multi-segmented Se-Te-Se nanorod system. The multi-segmented nanorods shows complex assembly behaviors due to the structural complexity and the difference in chemical affinity between different segments. We report that the solvent effect, surfactant effect which affect the assembly of the multi-segmented nanorod system.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Chemical Doping of Epitaxial Graphene by Triazine

박선민, 임희선, 이한길

숙명여대 화학과

The electronic structure of triazine adsorbed on epitaxial graphene (EG) was investigated using high resolution photoemission spectroscopy (HRPES). The measured work function changes verified that increased adsorption of the triazine on EG showed n-type doping characteristics due to charge transfer from triazine to graphene through the nitrogen. A double nitrogen bonding feature associated with the N 1s peak was clearly observed in the core-level spectra, indicating the presence of two different chemical environments.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Adsorption Configuration of Tyrosine on Ge(100)

양세나, 김예원, 이한길

숙명여대 화학과

The Adsorption structures of Tyrosine on Ge(100) surface have been investigated as a function of coverage using high-resolution photoemission spectroscopy (HRPES) and density functional (DFT) calculation. To converge these experimental and theoretical conclusion, we systematically performed HRPES measurements and DFT calculation for various coverage in the adsorption structures of tyrosine molecules on the Ge(100) surface. In this study, we found two different adsorption structure as a function of coverage in tyrosine on Ge(100), monitoring three core level spectra (C 1s, N 1s, and O 1s) using HRPES Through analysis of the binding energies, we confirmed that O-H dissociated and N dative-bonded structure emerges at low coverage (0.30 ML), which is the same to the result of glycine and alanine on Ge(100) system, whereas O-H dissociation structure also appears at higher coverage. Through the spectral analysis for tyrosine, we will demonstrate variation of coverage dependent structural change for tyrosine on Ge(100) surface using experimental (HRPES) and theoretical studies (DFT calculation).

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Development of MD simulation protocols for the non-natural cyclic crosslink in peptides using modified force field

홍주연, 함시현

숙명여대 화학과

Recent works have been shown that the incorporation of all-hydrocarbon cyclic crosslink to peptide backbone can greatly increase helical content of peptide, leading to an improvement in pharmaceutical properties. Herein, we report the development of several simulation protocols to properly generate force field for the non-natural cyclic crosslink in peptides.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Molecular insights into the effect of stereochemistry of the staples in the stabilization of α-helix: MD simulations study

홍주연, 함시현

숙명여대 화학과

Recent studies have shown that polypeptides bearing all-hydrocarbon crosslink (staple) can exhibit greatly increased α-helical contents, binding ability for their target receptors, and cell permeability. In particular, SS stapling system with i,i+4 crosslink performs preferentially over other combinations of stereochemistry with higher α-helicity. Herein, the molecular dynamics simulation results will be presented to understand the details of structural and thermodynamic behaviors for stapled peptides with different stereochemistry at a molecular level.

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Toward an Understanding of Pyrophosphate Hydrolysis: Quantum Mechanics calculation

홍주연, 함시현

숙명여대 화학과

Ab initio quantum mechanical methods were employed to study pyrophosphoric acid (H4P2O7) with different charged states (-3, -2, -1, 0). The equilibrium conformations in a gas phase and an aqueous phase were carefully located to understand the structures and reactions of pyrophosphates.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Molecular Simulation of Benzene Adsorption in MCM-41

문성두

부경대 화학과

The adsorption properties of benzene in MCM-41 with heterogeneous and cylindrical pore have been studied using grand canonical ensemble Monte Carlo simulation. Adsorption isotherm, average potential of adsorbate, and number density of molecules in MCM-41 were calculated, The simulated isotherms were compared with experimental ones, and different adsorption behaviors in MCM-41 with pore diameter of 2.2 and 3.2 nm were discussed. The simulated adsorption amounts above the capillary-condensation pressure agreed with the experimental ones. The results also showed that most of the molecular planes were nearly parallel to the pore axis. This orientation was not affected by the molecular position in the pore. The molecular planes were nearly parallel to the pore surface close to the pore wall.

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Size control of silver nanoparticles in poly-ol synthesis

한현숙, 김상호

공주대 화학과

The synthesis of silver nanoparticles with well-controlled size is very important in many practical applications. Especially in so-called poly-ol synthesis, the size and its distribution should be dependent upon many factors including the reaction temperature, precursor and surfactant concentration, reduction potential and viscosity of poly-ols. Here, we report a simple method to control the size of silver nanoparticles by using the poly-ol with different chain length and the reaction temperature. Further we suggest a possible nanoparticle formation mechanism in poly-ol synthesis based on the viscosity of poly-ols and the seed formation at different reaction temperatures.

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발표분야: 물리화학

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Structural Dynamics of RAS Oncoprotein and its interactions with Effector PI3Kinase Using Molecular Dynamics Simulations

박미래, 함시현

숙명여대 화학과

Ras protein is a signal-transducing small GTPase that plays central roles in the control of cell growth and differentiation. Ras oncogene is one of the famous oncogenes, and mutated Ras leads to oncogenesis and eventually cancer. Also, it has been suggested that the phosphoinositide 3-kinase (PI3K) is the primary oncogenic effectors of Ras signaling of many different effectors pathways. As we focused to Ras and its effector PI3K, we report structural dynamics and characteristics of Ras and PI3K using molecular dynamics simulation to provide thermodynamic properties of the binding intereactions between Ras and PI3K.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Understanding Structural Dynamics of Myc/Max Transcription Factor

박미래, 함시현

숙명여대 화학과

Myc as a transcription factor has been shown to play a critical role in control of cell growth, differentiation, and apoptosis. Deregulated expression of Myc occurs in a broad range of human cancers. Moreover, Myc dimerizes with Max as well as with a specific DNA (E-box), which is essential for the oncogenic function of Myc. Although the crystal structure of Myc/Max complex has been reported, the structural dynamics have yet to be investigated with an atomic resolution. Here, we have investigated conformational dynamics and characteristics of Myc monomer and of Myc heterodimer with Max using molecular dynamics simulation in explicit water.

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Silver and gold nanoparticles in water produced by laser ablation

김국기, 박승민

경희대 화학과

In the past years, laser ablation synthesis in solution emerged as a reliable alternative to traditional chemical reduction methods for obtaining metal nanoparticles. Laser ablation synthesis in solution is environment-friendly technique for synthesis of stable metar nanoparticles in water. We prepared silver and gold colloids by laser ablation of pure metals in water. SERS spectra could be obtained using these metal colloids.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 목 15:00~17:00

optical time of flight studies on the laser ablation of titanium target in N2 atmosphere

장윤주, 박승민

경희대 화학과

The interest of laser plasma with solid target has been widely studied. Laser ablation of a Ti target was attempted to investigate the formation mechanims and expansion dynamics of ions species including TiN cluster ions in the plume. Time-of-arrival distributions of ions were analysed to obtain their mean velocities and spatial distribution. optimisation and control of pulsed laser reative deposition of Ti in nitrogen atmoshere require the understanding of the plasma formation, gar pressure effect and the distance. in this contribution, time and space resolved emission spectroscopy and ion material were used to study the plasma dynamics in nitrogen gas atmosphere

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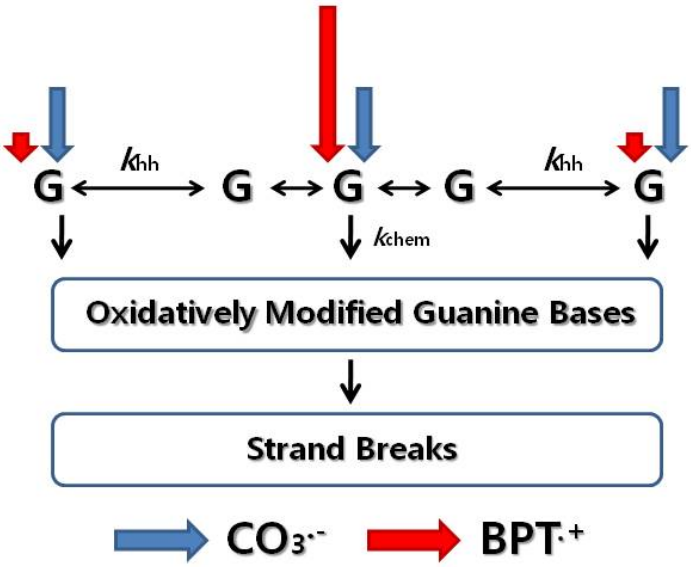
발표종류: 포스터, 발표일시: 목 15:00~17:00

Oxidation of Guanine in runs of G Sequence Contexts by Carbonate and Aromatic Pyrenyl Radicals: Relationship between Kinetics and Distribution of Alkali-labile Lesions

서유진, 이영애, 황길태

경북대 화학과

Carbonate radical anions(CO3·-) are potentially important oxidants of nucleic acids in living systems. These radicals can oxidize guanine bases in DNA through a one-electron transfer reaction process that ultimately results in the formation of stable guanine oxidation products (predominantly determined as the formation of diastereomeric spiroiminodihydantoin(Sp) lesions). There is growing evidence that, in vivo, these radicals are generated in reactions of peroxynitrite with carbon dioxide. However, the mechanisms of reaction of carbonate radical anions with nucleic acids are poorly understood. Therefore We have investigated reaction mechanisms, starting with a spectroscopic study of the kinetics of electron transfer from 20-35mer double stranded oligonucleotides to CO3·- radicals together with the effects of base sequence on the formation of the end-products in runs of one(G), two(GG), or three(GGG) contiguous guanines. The distributions of alkali-labile guanine lesions induced by CO3·- or BPT radicals in different sequence contexts have been analyzed by gel electrophoresis. The impact of base sequence on the yield of oxidative DNA damage induced CO3·- or BPT radicals will be discussed.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

Time-Resolved IR study of cyano cytochrome c

김주영, 임만호, 박재홍, 이태곤

부산대 화학과

We measured the rebinding dynamics of the ferric CN complex of cytochrome c (cytcCN) in D_2O at 293 K using femtosecond vibrational spectroscopy. CytcCN was prepared by horse heart cytochrome c (cytc) adding 10-fold escess of potassium cyanide. Upon UV excitation of CN-ligated cytochrome c at 570 nm, the transient infrared spectra show a strong bleach of the cytcCN stretching band near 2120 cm^{-1}, as well as two smaller absorption features, one immediately is to the red of the bleach (band1) that is from incresed vibrational temperature in the protein, which shifts the CN transition to lower energy, and the other is red-shifted by ~ 30 $^{-1}$(band2). Since free CN- and HCN bands are 3~5 times weeker than heme-bound CN and spectral position is also similar as heme-bound CN. However, anisotropy signal doesn't show any change of CN angle against heme plan. therefore CN associated band2 doesn't from CN dissociation. It could be either loosely bound stretching mode or vibrational excitation.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Aminolyses of Bis-Methyl Z-Substituted Thiophenyl Phosphates in Dimethylsulfoxide

Adhikary Keshab Kumar, *Hasi Rani, 김찬경, **이본수, 이해황

*인하대 화학과 *인하대 물리화학과 **인하대 총장실*

The mechanistic interpretation with its statistical database of physical behavior of organo-phosphorus compounds are appearing as an interesting, informative and challenging recently in the field of biochemistry, microbiology and physical organic chemistry. In the incessant of the progress of the search, we have investigated the kinetics and concern physical factors of pyridinolysis of bis-methyl Z-substituted-phenylthiophosphates in dimethylsulfoxide at 35.0oC. Usually a biphasic Hammett plot indicates the mechanistic alteration during the change in X or Z-substituents variation of nucleophiles or substrate respectively while acting in the reaction stream or linear correlation for straightforward SN1 or SN2 type of mechanistic interpretation. The deuterium kinetic isotope effect is the strong tool for mechanistic interpretation for a long and we have taken its advantage to extent the mechanistic criteria for the current system, although respective activation parameters and obtained cross-interaction constants are the main basic information for interpreting mechanism. Where, we are especially endeavored to introduce the frontal and backward attack of nucleophiles through the usual SN1 or SN2 nucleophilic substitution reaction. In the present work, we intended to speculate and provoke the mechanistic criteria from the Hammett and Brönsted correlations in the course of reactions mentioned above.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Colloidal 'Non-toxic' Quantum Dots by Pyrolysis Method

박영롱, 원나연, 김성지

포항공과대 화학과

Quantum dots (QDs) can be a promising fluorescent marker in biological imaging applications due to the unique optical properties such as high extinction coefficient, high quantum yield, broad absorption, and narrow and symmetric emission profiles. Typical QDs may contain toxic elements such as Cd, Pb, Hg, or As. This inherently limits QDs from potentially being widely used for medical or biological applications. High quality 'non-toxic' QDs were synthesized that include InP and CuInS2 QDs. The solvent and QD precursors were judiciously chosen to obtain highly bright and stable QDs with reproducible manner. For example, high quality InP QDs were obtained by means of a simple one-pot synthesis in the presence of polyethylene glycol (PEG). PEG is cost-effective and is proven almost non-toxic in human physiology. The PEG is also recyclable; can be easily recovered after synthesis by simple physical separation. Various precursors which are relatively inexpensive and non-toxic were tested for InP and CuInS2 QD syntheses. The new 'non-toxic' QDs synthetic methods can promise environmentally friendly display device and biological imaging applications.

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Near-Infrared Multiplexed In Vivo and In Vitro Imaging using Quantum Dots and Inorganic Nanocrystals with Lanthanide Ions

정상화, 원나연, 김성지

포항공과대 화학과

Quantum dots (QDs) have the potential for bioimaging contrast agents by bright luminescence, resistance against photobleaching, and tunable emission wavelengths. Lanthanide-doped nanoparticles (LNs) can have advantages in bioimaging applications due to their narrow emission bandwidth, nonblinking, and relatively low toxicity. Both QD and LN can emit at near-infrared (NIR) wavelengths which can provide maximal tissue penetrations from the minimal interferences by water and biomolecules and from the reduced auto-fluorescence. Multiplexed imaging provides the opportunity to investigate the complex biological phenomena governed by multiple biomolecules. QDs with different emission wavelengths can be multiplexed by single excitation light. Multiplexing between QDs and LNs can be obtained by switching the excitation sources while they emit at same wavelength domain. NIR emitting QDs and LNs were synthesized with judicious emission wavelength control by pyrolysis method to expand the multiplexing capability in 700 to 900 nm. Using small animal models, in vivo real-time multiplexed imaging will be demonstrated with QDs and LNs simultaneously and complimentarily exploited for the contrast agents.

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Exploration of the potential energy surface for the loss of HCN from ionized pyridine

임민경, 최중철

동국대 화학과

The potential energy surface (PES) was explored for the loss of HCN from pyridine molecular ion. Quantum chemical calculations were carried out with the G3//B3LYP method. We obtained the pathways for the formation of four isomeric C_4H_4+ ions; butatriene, cyclobutadiene, methylenecyclopropene, and vinylacetylene molecular ions. The RRKM analysis was performed on the basis of the obtained PES to predict the dissociation rate constant and the branching ratio of the productC_4H_4+ ions.

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Dissociaton of pyridazine, pyrimidine, and pyrazine molecular ions : A theoretical study

정선화, 김선영, 최중철

동국대 화학과

We have explored the potential energy surfaces (PESs) for the isomerizations and dissociations of pyridazine, pyrimidine, and pyrazine molecular ions. Several pathways were found using quntum chemical calculations at the G3//B3LYP level. The H shifts followed by ring opening were the important mechanisms for the loss of HCN, HNC, N_2, or $HN_2^{\cdot}$. Based on the PESs obtained, the dissociation kinetics will be discussed.

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Hydrothermal reaction of CuO nanostructures in various alcohols

차병관, 김재욱, 지명진, 권태필, 박병천, 경동현, 김종규

단국대 화학과

This study has been demonstrated to be very useful to understand a hydrothermal method of crystalline copper oxide(CuO) nanostructures by simple, that is been successfully prepared by solvent of various alcohols. By resulting solvothermal reaction of copper acetate in various alcohols, The manufacture of copper oxide(CuO) powder was formed. In this current study, the effects of reaction on the product morphology as well as crystallization mechanism were examined by using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) techniques. It was found that size of the nanoparticles were changed in various alcohols.

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Morphologies of zinc oxide on the different alkali metal and hydroxyl group

박병천, 김재욱, 차병관, 지명진, 권태필, 진훈열, 김종규

단국대 화학과

In this study, three alkali metals (lithium, sodium, potassium) and hydroxyl group were investigated in morphology of zinc oxide (ZnO). To using the mixture solution of the three alkali metals and the hydroxyl group as solvent, the zinc oxide has been prepared for the hydrothermal synthesis. The variation of morphologies has been considered by influence of different concentration of alkaline solution and also it was changed by between zinc species and hydroxyl group. Alkali solutions play crucial role in morphological control of ZnO structure. The structure and morphology of as-prepared samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM).

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Growth of Carbon Nanotube by Microwave Plasma Enhanced Chemical Vapor Deposition(MPECVD) using Nickel Catalyst

허창순, 이상국

부산대 화학과

We investigated the growth process of petal-like carbon nanowalls (PCNWs) on a Si substrate bymicrowave plasma-enhanced chemical vapor deposition (MPECVD). It is revealed that the PCNWs aregrown at the fine-textured structure on the Si and the growth process does not require the catalyst. ThePCNW initially has a semicircular shape. The height, thickness, and mesh size increase with growth time.In the case using C_2H_2/H_2 system, aligned petal-like carbon nanowalls (PCNWs) were grown verticallyon the substrate. It is found that the height of PCNWs as a function of time obeys the square root law.Scanning electron miscroscopy (SEM), energy-dispersive spectroscopy (EDS), and atomic forcemicroscopy (AFM) were used to analyze the CNT morphology and composition.

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Solvation Thermodynamics Analysis of Amyloid-Beta Protein

정성호, 이제욱, 함시현

숙명여대 화학과

Aggregation of Amyloid-beta (Ab) proteins has been implicated as a primary cause of Alzheimer's disease, but the mechanism for the aggregation still remains elusive. The major drving force for the protein self assembly is believed to be hydrophobic collapse followed by nucleation dependent association between aggregation-prone states of Ab proteins. Recently, hydrophilic contribution based on the main chain hydrogen bonding has been proposed in correlation with the dehydration of backbone. To corroborate this proposal, thermodynamics analyses in terms of the protein intramolecular energy, hydration energy, and hydration entropy are performed. In this presentation, we will report the results of such analyses on Ab protein which are obtained by combining the molecular dynamics simulations with the integral equation theory of liquids.

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Conformational Preferences and pK_a Value of Selenocysteine Residue

변병진, 강영기

충북대 화학과

L-Selenocysteine (Sec), an analogue of L-cysteine (Cys), where sulfur is replaced by selenium, is the known as the twenty-first amino acid. Incorporation of Sec into selenoproteins requires a specific mechanism to decode the UGA codon in mRNA, which is one of the normal termination codons for translation. The conformational preferences of the Sec dipeptides with the selenol and selenolate groups (Ac-Sec-NHMe and Ac-Sec$^-$-NHMe, respectively) and the apparent (i.e., macroscopic) pK_a value of the Sec dipeptide are studied at the dispersion-corrected density functionals B2PLYP-D/6-311++G(d,p)//M06-2X/6-31+G(d) level of theory in the gas phase and with the implicit SMD solvation model in water. The conformational analysis indicates that the Sec and Sec$^-$ dipeptides have different conformational preferences from the Cys and Cys$^-$ dipeptides in water, respectively, although in the gas phase their most stable structures are same as those of the Cys and Cys$^-$ dipeptides. The pK_a value of the Sec residue is calculated to be 5.47 at 25 °C using the statistically weighted free energies of all feasible conformations for the Sec and Sec$^-$ dipeptides in the gas phase and solvation free energies, which is consistent with the observed value of 5.43 ± 0.02.This work was supported by the grant of the Korean Ministry of Education, Science and Technology (The Regional Core Research Program/Chungbuk BIT Research-Oriented University Consortium).

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Emission Behavoir of the Naphthalic Amide Derivatives having the Inductive Ending Group

Minh Phung Doan, 정우철, *전기석, 이기환, **최창식

*공주대 화학과 *한국화학연구원 나노바이오융합연구센터 **극동대 한약자원학과*

The aromatic conjugated imine or imide systems were previously reported toward the development of the emissive photo-materials, photo-sensing and photo-switching ones. Various functional parts were introduced into the structural architecture to develop the smart and highly emissive photo-materials. The aromatic conjugated amide systems were recently prepared to compare with the compounds reported previously. Those emission behavior will be discussed systematically.

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Time-resolved reaction of CN radical in $CHCl_3$

이태곤, 박재홍, 김주영, 임만호

부산대 화학과

In condensed phase, photodissociated fragment undergoes reaction with solvent. CN radical from ICN can abstract H or Cl, substitute in $CHCl_3$. ClCN and HCN is investigated in previous studies. HCN has three vibrational modes, and we measured C-H (3265 / 3160 cm^{-1}) and C-N (2093 / 2067 / 2042 cm^{-1}) stretching modes. In equilibrium spectrum of HCN, amplitude of C-H stretching band is 15 times bigger than C-N stretching. But in our data, C-N / C-H amplitude ratio is smaller than 2, so we quoted linear / bridge complex. Vibrational modes of HCN and complex make us to establish more detailed kinetic model of HCN. $CHCl_2CN$ and CCl_3CN for substitution reaction, their extinction coefficient of C-N stretching mode is 1.3 $M^{-1}cm^{-1}$ and 10 $M^{-1}cm^{-1}$. This value is too low, so we couldn't measured substitution reactions.

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Synthesis of TiO_2 Nanopearls and Nanorices: Visible-Light Photocatalysis

배은주, 윤민중

충남대 화학과

New TiO_2 was synthesized by the hydrothermal processing in acid and base solutions. The structure of as-synthesized TiO_2 nanostructures were characterized by measuring x-ray diffraction (XRD) patterns, scanning electron microscopy (SEM), transmission electron microscopy (TEM) images and Brunauer-Emmett-Teller (BET) surface areas. These results proved that the as-prepared TiO_2 nanomaterials have shapes of nanopearls and nanorices of anatase phase. Their UV-visible reflectance absorption spectra were observed to have low band gap energy (3.03 and 3.07 eV, respectively), exhibiting surface absorption band in the visible range from 400 to 600 nm. The degradation of methylene blue (MB) over the as-prepared TiO_2 nanomaterials was observed upon visible-light irradiation, which was found to be very efficient as compared with any other conventional visible-light responsive TiO_2 nanostructures.

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Triad TiO_2 Nano-Bio Composites. A Candidate of Solar Cell

이형주, 윤민중

충남대 화학과

TiO_2 nanomaterials have been widely studied as important substrate for solar cells. However due to its wide bandgap, it can only be activated by near-UV radiation, not by visible light which is dominant in the solar radiation. The sensitisation of TiO_2 with a wide variety of inorganic and organic dyes for light harvesting has been investigated over the last 20 years for the development of efficient solar cells. Given their efficacy in photosynthesis, porphyrin dyes have great potential in this regard. And the DNA provides the electron that can increase efficiency by using. Thus, in this work nitrogen-doped TiO_2 nanochains coupled with silver ion (Ag^+-N-TiO_2 nanochain) was formed, followed by adsorption with porphyrine(TTCP; Tetrakis(4-caboxyphenyl) porphyrin) or TMS - porphyrin and DNA(polyG-C·polyG-C, polyA-T·polyA-T) to fabricate the triad TiO_2 nanobio composites. It was found that the photoelectric conversion efficiency of the composite was highly improved depending on DNA base pairs and porphyrin shape.

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Surface Properties of Charged Cathode Materials for Li-Ion Batteries

박연주, 김남훈, *최현철, 정영미

*강원대 화학과 *전남대 화학과*

Rechargeable Li-ion batteries have become the most promising power sources for a variety of portable electronic devices. Therefore the improvement of Li-ion batteries safety is one of the key issues. Recently, the influence of electrolyte additives content on the cathode surface and electrochemical performance of the cathode materials have been studied. In order to improve the Li-ion batteries safety, we have investigated the cathode surface under high voltage conditions by SEM, Raman and XPS and have proposed mechanism of solid electrolyte interface (SEI) formation by 2D correlation spectroscopy.In this presentation, we have studied the surface properties of the charged cathode materials with and without electrolyte additives. The effect of electrolyte additives on surface reaction of cathode materials under high voltage conditions will be discussed in more detail.

Acknowledgement
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다공성 알루미나를 이용한 Ni 전착과 모델촉매에 대한 연구

조춘식, 김창민

경북대 화학과

일정한 크기의 구멍으로 이루어진 AAO(Anodic Aluminum Oxide) 템플릿을 이용하여 다양한 분야에 이용 될 수 있는 나노 닷, 나노 와이어를 만들 수 있다. 본 연구 에서는 AAO 를 이용한 금속 나노 촉매를 합성 하였다.잘 정렬된 구멍의 크기와 배열의 일정함을 유지 하기 위해 실험 단계에 적절한 어닐링 작업과 용액을 통한 화학적 연마, 에칭, 가열 작업이 동반되었다. 알루미늄 양극 산화시 약 273K 에서 0.3M 옥살산과 3% 황산을 이용하여 각각 50V, 40V 와 10V 전압을 일차 산화, 이차 산화시 걸어주어 70~80nm 와 30nm 의 구멍을 만들었다.이렇게 완성된 다공성 알루미나를 주형틀로 이용하여 Ni 전착에 성공 하였으며, Ni/Al203 모델 촉매로 이용하여 탄화수소 분해 반응에 이용할 계획이다.

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Zincon as Resonance Raman Probe for Protein Concentration Determination

Lei Chen, *박연주, *서형균, *홍원진, *정영미, **Bing Zhao**

*State Key Laboratory of Supramolecular Structure and Materials, Jilin University *강원대 화학과*

Resonance Raman spectroscopy (RRS), which can enhance Raman signal by 10^4-10^6 times than normal Raman spectroscopy, is a powerful approach to characterize structures of biomolecules at low concentrations. As a colorimetric reagent, zincon has been widely used in metal ion detection. In the Bradford method, when zincon bind to protein, their absorbance show red shift (from 465 nm) and broadened. The proposed method for total protein detection is based on resonance Raman of unbound zincon to the protein. Intensity of zincon as a resonance Raman probe increase with protein concentration decreased. This proposed method can be applied to lower protein concentration detection. Their lower detection limits demonstrate its great potential in low abundance detection, and zincon as resonance Raman label would be useful for the detection of proteins and protein mixture in proteomic studies.

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Polyynes formed of by pulsed laser ablation of graphite in aqueous media

신승근, 박승민

경희대 화학과

Polyynes were prepared by liquid-phase laser ablation of a graphite target at 1064 nm and identified by analyzing UV absorption spectra. We observed that major UV absorption peaks coincide with the electronic transitions corresponding to linear hydrogen-capped polyynes (CnH2: n = 6, 8, 10). The peak intensities increased when polyynes were produced by irradiating the target immersed in acidic media, while those were relatively weak in basic media.

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Bending and Flexibility of Methylated and Unmethylated DNA Detected by Fluorescence Resonance Energy Transfer

김지아, *이상학, **김성근

*서울대 화학과 *서울대 화학부 **서울대 화학부&생물물리 및 화학생물학과*

The methylation of DNA affects nucleosome formation and its positioning in chromatin,giving rise to a significant change in DNA structure. DNA methylation typically occurs at thenumber 5 carbon of cytosine within the context of CpG dinucleotide, and is known to playa critical role in epigenetics, with consequences in gene regulation, cellular differentiation,and even carcinogenesis. However, much is unknown about the effect of DNA methylationon its mechanical properties and dynamics because of the difficulty in observing the changein DNA structure specifically caused by methylation. In this study, FRET-based approach isadopted to examine the bending and flexibility of methylated vs. unmethylated DNA at theensemble and single-molecule level.

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Single-molecule Study for the Conformation-dependant Toxicityof Amyloid (α-synuclein) Oligomers

허현, *김성근

*서울대 화학부 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

Parkinson's disease (PD) is one of the neuro-degenerative diseases that heavily affect the aged population and those with genetic mutation. Protein aggregation via pre-fibrils with cytotoxicity on the neuronal cell is commonly observed in the PD patients including sporadic and familial cases. We investigated the structural change of amyloid monomers on their way to oligomers using single-molecule FRET and FT-IR spectroscopy. We found that α-synuclein oligomer has a hydrophobic interaction with the lipid membrane, which leads to the formation of nano-pore structures on the membrane in vitro.

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Single-molecule Fluorescence Assay Reveals Dissociation Dynamicsof DNA Polymerase on the Lagging Strand of DNA

임영빈, *김성근

*서울대 생물물리 및 화학생물과 *서울대 화학부, 서울대 생물물리 및 화학생물과*

It is well known that DNA polymerase (DNAP) undergoes various motions such as stalling, stopping, positional exchange, and dissociation during DNA replication, but its motional dynamics is still largely unknown. To examine detailed motions of DNAP on the lagging strand of DNA, we adopted single-molecule fluorescence assay that utilizes the fluorescence enhancement of the Cy3 dye upon environmental changes. By monitoring the fluorescence intensity of a single Cy3 dye in real time, we were able to observe dynamical motions of DNAP on DNA template strands. We investigated the motional responses of DNAP when it meets a primer on the lagging strand to address the effect of a primer blockade. This technique should allow us to elucidate the intrinsic motional behaviors of DNAP on a DNA strand at the single-molecule level.

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Relation between Quantum and Classical Diffusion Coefficients

김태준, 김효준

동아대 화학과

We study the general solutions regarding the evaluation of quantum mechanical time correlation functions. In this presentation, we introduce the quantum correction approach to utilize the general relation between quantum and classical correlation functions. The quantum corrected correlation function only requires classical correlation functions and their derivatives with respect to time. We investigate quantum mechanical effects on diffusion constants of liquid argon and neon from classical molecular dynamics simulations and compare classical diffusion constants with quantum diffusion constants. We find that the difference between classical and quantum diffusion constants is bigger for the higher density. For high density liquids, quantum effects on diffusion constants should not be neglected.

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Monte Carlo Simulation for the Diffusion in Condensed Phases

김형희, 김태준, 김효준

동아대 화학과

Monte Carlo simulation results for the diffusion in condensed phases will be presented. We study the fundamental phenomena of diffusive motions using lattice-based Monte Carlo simulations to improve utilities of simulations for the applications to complex real systems. The random walk on irregular lattices has attracted increasing attentions since it can represent numerous complicated diffusion-reaction systems such as *in vivo* biological reactions and percolation clusters. We report amusing results of diffusive motions in irregular spatial systems, which are useful to explain anomalous motions in a high degree of molecular crowding environments.

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Mesoporous Silica-pillared Layered Silicate as Catalytic Support for Partial Oxidation of Methane

박경원, 정종화

경상대 화학과

Highly ordered mesoporous silica-pillared kenyaite (SPK) and magadiite (SPM) were prepared by the hydrolysis of tetraethylorthosilicate (TEOS) through the catalytic effects of dodecylamine (DDA) in the interlayer space. SPM and SPK exhibited regular gallery heights of 3.0 and 3.4 nm, narrow pore size distributions of 2.5 and 3.0 nm and large specific surface areas of 877 and 1029 m^2/g, respectively. The sharpness of the d 00l peak for SPK was well-preserved even after heating up to 800 °C in air, while the peak for SPM collapsed between 700 and 800 °C. A uniform spacing of 2-3 nm between the layers were obtained from the TEM images of SPM and SPK. SPK and SPM impregnated with 5 wt% of Ni and Pd were examined as potential catalysts in the partial oxidation of methane at 750 °C. The Ni/SPK, Ni/SPM and Pd/SPK catalysts showed higher methane conversions, which remained stable for almost 100 h of heating. Especially, the Pd/SPK catalyst exhibited high selectivity and stability to H^2. The results indicate that the SPK and SPM products are highly applicable as catalytic supports in high temperature reactions.

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Fabrication of UV curing resin polymer gel electrolytes for DSSC

박근우, 유수련, 서형균, *정재원, **황철균, 정영미

*강원대 화학과 *한국이엔에쓰(주) **나노융합실용화센터 나노융합개발팀*

The development of renewable energy sources for future energy systems, especially solar energy, has been growing at an ever increasing pace due to global warming and limited availability of fossil fuels. The dye-sensitized solar cell (DSSC) provides an attractive alternative to solid-state photovoltaics for the conversion of solar energy to electricity. Especially in light of their potential low cost compared to conventional silicon-based solar cells. DSSC based on TiO_2 as the nanostructured electrode are capable of achieving efficiencies of 11%. The high efficiency, however, can be obtained only when employing volatile electrolytes, which commonly have some restrictions in guaranteeing stability. For the practical application of DSSCs, electrolytes with reliable stability, as well as high efficiency, are highly demanded. In this study, a series of UV curing resin gel polymer electrolytes has been prepared by varying the concentration of UV curing resin. Details of characterization of a new gel polymer electrolyte based on UV curing resin and its efficiency for DSSC will be discussed.

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SERS Immunoassay Using Patterned Gold Particles Substrate

서형균, 홍원진, 정영미

강원대 화학과

Surface-enhanced Raman scattering (SERS) has received much attention due to its considerable potential in high selective and sensitive detection of molecules of interest even in single molecular detection. SERS has been a promising candidate for various applications in chemical-biochemical analysis, nanostructure characterization and biomedical applications. Especially, SERS immunoassays based on antigen-antibody bonding have been studied for biomarkers for early cancer diagnosis. PSA, which is a glycoprotein consisting one polypeptide chain, has been used as a serologic marker for detecting prostate cancer. In this study, the sandwich type SERS immunoassay was used to detect PSA. To capture PSA antigens onto the immobilized layer of antibodies on the gold substrate, we prepared a monolayer of gold nanoparticles on the APTMS-derivatized surface of a glass slide by using the SAM technique, which was patterned by micro-contact printing method. This SERS immunoassay method can be applied successfully for biosensing. Details of the SERS immunoassay and SERS images will be discussed.

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Characterization of biodegradable spin-coated films of polymer blends by 2D-IR Correlation spectroscopy

김민경, 유수련, *Isao Noda, 정영미

*강원대 화학과 *Procter & Gamble Company*

Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (P(HB-co-HHx)), which is a new member of the polyhydroxyalkanoate (PHA) family, has been studied extensively. We have recently investigated thermal behavior of spin-coated films of PHB-co-HHx copolymers. It is also important to investigate the thermal behavior of P(HB-co-HHx) in the presence of other polymers like PEG. P(HB-co-HHx) is fully miscible with poly(ethylene glycol) (PEG). In this study, P(HB-co-HHx) blends with a PEG content of 2, 10, and 20 wt% were prepared from chloroform solution. Crystallization of spin-coated films of P(HB-co-HHx)/PEG blends are investigated by 2D correlation spectroscopy. Details of 2D correlation spectra of spin-coated films of P(HB-co-HHx)/PEG blends will be discussed.

Acknowledgments
This work was supported by National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0065428) and the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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Charge Transfer Dynamics of InP and InP/ZnS NanocrystalsStudied by Femtosecond Transient Absorption Spectroscopy

양일승, *강준희, **장은주, **전신애, **장효숙, ***김성근

*서울대 화학부 *서울대 생물물리 및 화학생물학과 **삼성종합기술원 Advanced Materials ***서울대 화학부 & 생물물리 및 화학생물학과*

Synthesis of Type III-V semiconductor nanocrystals has recently drawn a great deal of interest due to their reduced toxicity compared with Type II-VI and IV-VI nanocrystals. In particular, indium phosphide (InP) has been studied extensively owing to its ease of synthesis. Passivation of semiconductor nanocrystals such as InP is reported to increase the quantum efficiency and stabilize its structure by protecting the core from external environments. We investigated the charge transfer dynamics of InP nanocrystals passivated with zinc sulfide (ZnS) by using femtosecond transient absorption and time-correlated single photon counting spectroscopy.

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The Determination of Total Integral Cross Sections Involving States Coupled by Conical Intersections for Electron Photodetachment and Photoionization of Polyatomic Molecules

한승석

명지대 화학과

The formal underpinning is derived for the computational determination of electron photodetachment and photoionization total integral cross sections for molecules in which the residual species, which can be a neutral or an ion, has states that are strongly coupled by conical intersections. The theory takes full account of the requisite antisymmetry of all the electrons and the potential nonorthogonality of the orbital for the scattering electron to the occupied molecular orbitals of the residual. The breakdown of the Born-Oppenheimer approximation requires significant modifications to the standard adiabatic state theory. The developed theory builds on ideas from theories of low energy electron scattering, in which the scattered electron is described by an orbital taken as channel dependent but independent of nuclear coordinates. The derived computational approach is based on the accurate description of the vibronic levels of the residual species using the nonadiabatic vibronic coupling theory of Koppel, Domcke and Cederbaum. The electron scattering problem is solved using the complex rotation L^2 method of Han and Reinhardt. This approach has the advantage that both Coulomb and free electron boundary conditions can be treated in the same approach.

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Water-Soluble Ultra-Small Manganese Oxide Surface Doped Gadolinium Oxide Nanoparticles for T_1 MRI Contrast Agent

박자영, *최은숙, **Kattel Krishna, Xu Wenlong,** 김한결, 이은정, **ANIL PATEL,** 이강호

*경북대 화학과 *국립암센터 분자영상치료연구*

We have developed ultra-small gadolinium oxide nanoparticles, which are surface-doped with manganese oxide. The surface-doped nanoparticles ranged from 1 to 2 nm in diameter. They were further coated with hydrophilic biocompatible lactobionic acid. In-vitro tests of the sample solution indicated clear dose-dependent contrast enhancements in both T_1 and T_2 map images, showing that the nanoparticles may be used as both T_1 and T_2 MRI contrast agents. Their performance as a T_1 MRI contrast agent was proved in vivo through T_1 MR images of a mouse.

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Synthesis, characterization and in vivo study of antibody conjugated gadolinium oxide nanoparticles

이은정, ANIL PATEL, 박자영, Kattel Krishna, Xu Wenlong, 김한결, 이강호

경북대 화학과

We have synthesized PEG diacid surface modified gadolinium oxide nanoparticles and characterized by HRTEM and FT-IR. The conjugation of this nanoparticle with different antibody viz. AMFR (autocrine motility factor receptor) and AFP (α-fetoprotein) antibody was carried out by carbodiimide chemistry. The synthesis of both AMFR (autocrine motility factor receptor) and AFP (α-fetoprotein) antibody conjugated to gadolinium oxide nanoparticles also carried out by same technique. To verify the conjugation of the antibody to particle surface, samples were conjugated with fluorescently (FITC) lableled secondary antibody. The samples were analyzed with flow cytometer and results were compare with control sample. In vivo study of antibody conjugated gadolinium oxide nanoparticles was also carried out.

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Surface modification and dispersion process development of nano metallic powder

김한결, 이은정, 박자영, **Kattel Krishna, Xu Wenlong, ANIL PATEL,** 이강호

경북대 화학과

금속나노분말소재는 미래 나노기술의 핵심소재로 전기, 전자, 환경, 에너지, 건축, 의료 등 다양한 IT/ET 분야에 활용이 기대되는 소재이다. 우리는 금속나노분말의 다양한 활용을 위해서 금속나노입자의 표면개질을 통해 분산성을 증대하여 안정한 콜로이드 용액을 만들고자한다. 금속나노분말의 표면개질을 위해서 isobornyl acrylate, 2-propanol, terpineol 등의 유기용매를 사용하였고, 유기용매를 다양한 종류의 분산제와 금속 나노 분말을 일정 비율로 혼합하고 볼밀 기기를 이용하여 안정한 콜로이드 용액을 제조한다. 분산제로는 폴리머, 계면활성제 등을 사용하고 분산제 첨가량, milling time, milling speed 등에 따른 분산 안정성과 특성을 알아내고 최적 조건을 찾고자 한다. 금속나노입자의 분산 안정성을 평가하기 위해 DLS, TEM, Turbiscan 장비를 사용할 것이다. 최종적으로는 최적의 분산제 발굴 및 분산기술을 활용하여 금속나노분말의 제품화에 적용하는데 그 목적이 있다.

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Synthesis and characterization of D-glucuronic acid coated lanthanide oxide nanoparticles for magnetic resonance imaging (MRI)

Kattel Krishna, 박자영, **Xu Wenlong**, 김한결, 이은정, **ANIL PATEL**, 이강호

경북대 화학과

We developed a simple one-step synthesis of D-Glucuronic acid surface-modified ultra small LnO nanoparticles.They were characterized by using MP-XRD ,TEM, FT-IR spectrophotometer,TGA,SQUID magnetometer and Magnetic Resonance Imaging(MRI) instrument. The resulting data suggest that ligand-coated ultra-small Ln_2O_3 nanoparticles will be extremely valuable for target specific biomedical applications such as MRI contrast agents.

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Rebinding dynamics of nitric oxide to metmyoglobin in water by femtosecond IR spectroscopy

박재홍, 이태곤, *박재헌, 임만호

*부산대 화학과 *포항공과대 포항가속기연구소/빔라인부*

We measured the rebinding dynamics of NO to ferrous Mb and found that most of NO geminately rebinds nonexponentially in 1 ns. Vibrational bands of NO in MbNO revealed two bands and kinetics of the rebinding of both bands are identical, indicating that the dynamics of geminate rebinding to ferrous Mb is conformation independent. Here we investigated NO rebinding dynamics to ferric Mb and compare it with that of ferrous Mb. Stretching mode of NO in ferric MbNO has two overlapping bands, main band at 1921 cm-1 and minor one at 1907 cm-1, suggesting that ferric MbNO has at least two conformational substates. The rebinding of NO to ferric Mb in D2O at 283 K is nonexponential. The decay of the main band is slower than that of ferrous MbNO band but almost complete in 1 ns, indicating that NO rebinding to the main conformation of ferric Mb is less efficient than ferrous Mb. The minor band does not decay in 1 ns, suggesting that the geminate rebinding of NO to the minor conformation of ferric Mb is negligible during 1 ns. The minor conformation is suggested to arise from the interaction of the protonated His 64 with NO. Clearly the structure of amino acid residues near the active site of the protein is very critical in controlling protein function (lignad binding).

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One-Pot Synthesis and SERS Characterization of Poly(ethylenimine)-Stabilized Au/Ag Alloy Nanoparticles

김지훈, 신권수, *김관

*숭실대 화학과 *서울대 화학부*

One-pot synthesis of Au/Ag alloy nanoparticles with controlled composition as well as pure Au and Ag nanoparticles has been developed using poly(ethylenimine) (PEI) as a reducing and a stabilizing agent simultaneously. UV/visible spectra suggest the formation of alloy nanopartucles in conformaty with the mole fractions of gold and silver used initially in preparing the alloy sols. The resulting PEI-stabilized Au/Ag alloy nanoparticles exhibit distinct surface-enhanced Raman scattering (SERS) signals with 632.8 nm radiation as the excitation source. We have confirmed that the SERS spectral feature of 2,6-dimethylphenyl isocyanide (2,6-DMPI) on pure Ag is distinctly different from that on pure Au. Furthermore, the SERS spectral feature of 2,6-DMPI on Au/Ag alloy particles, even with a nominal composition of 75% Au and 25% Ag, is the same as that on pure Ag. The present observation supports that the outermost layers of the PEI-stabilized Au/Ag alloy nanoparticles are highly enriched in Ag atoms compared with their interiors.

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Role of electron correlation in electrical anisotropy: Iron pnictide superconductors

지효석, 심지훈

포항공과대 화학과

Recently, iron pnictide superconductors are intensively studied due to its high temperature superconductivity and possible route for finding new type high Tc superconductors. Due to the electron correlation effect of Fe 3d orbitals, many experimental results show disagreement with conventional theoretical approaches such as density functional theory (DFT). In this study, we have investigated the electron correlation effect on the electronic structures of iron pnictide superconductor, especially LiFeAs, using the combination of DFT and dynamical mean field theory (DMFT). The computed k-resolved spectral functions are in good agreement with ARPES results. Also the calculated specific heat coefficient gamma is well consistent with the experimental result. Moreover, we found that different size of electron mass enhancement causes a considerable effect on the electronic anisotropies, and our result is in good agreement with recent experimental result. So we conclude the correlation effect on Fe d orbital has an important role in describing the electronic structure and anisotropy of iron pnictide superconductors.

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Synthesis of Poly(allyamine)-Stabilized Copper Nanoparticles and Their Applications in SERS and Catalysis

김인현, 신권수, *김관

*숭실대 화학과 *서울대 화학부*

Poly(allylamine) (PAAm)-stabilized spherical copper nanoparticles are synthesized by the reduction of copper(II) salt with hydrazine in aqueous solution under atmospheric air in the presence of PAAm capping agent. The advantage of this synthetic method is the production of water dispersible copper nanoparticles at room temperature under no inert atmosphere, making the synthesis more environmentally friendly. The size and shape of the copper nanoparticles can be controlled by changing the relative concentration of PAAm in the solution. The obtained copper nanoparticles have been characterized by UV/visible spectroscopy and transmission electron microscopy. The resulting copper nanoparticles show efficient surface-enhanced Raman scattering properties and can effectively catalyze reduction of 4-nitophenol by sodium borohydride in aqueous solution. These characteristics of the PAAm-stabilized copper nanoparticles can allow them to be highly promising substrates for a range of different analytical and catalytic applications.

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Magnetic and water proton relaxivity properties of gadolinium oxide nanoparticles

Xu Wenlong, Kattel Krishna, 박자영, 김한결, 이은정, ANIL PATEL, 이강호

경북대 화학과

Fluorescein and fluorescein isothiocyanate(FITC) surface-modified Gadolinium oxide nanoparticles synthesized in triethylene glycol were nearly monodisperse in diameter and highly water-dispersible. We report a facile one-pot synthesis and characterization with XRD, FT-IR, TGA, Fluorescence spectrometer, TEM, SQUID magnetometer, confocal imaging and MRI instrument. These nanoparticles can be used as MRI contrast agent as well as optical imaging. This dual imaging capability will increase the possibility of an early observation of disease such as cancer.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Developments of Corona Excited Supersonic Expansion Spectra of Transient Molecules

이승윤, 이상국

부산대 화학과

One of the most interesting subjects in physical chemistry is to determine the molecular structure of transient molecules which are believed to play very important roles in chemical reaction. For this purpose, there are many developments of spectroscopy. We have determined to develop a spectroscopic method for the vibronic emission spectra of transient molecules by employing a long-path double monochromator and a technique of corona excited supersonic expansion(CESE). The CESE system was consisted of corona discharge and supersonic free expansion with a home-made quartz nozzle which was modified from the original Engelking type. Using a CESE system, we get the spectra of N_2 and N_2 positive ion from the corona discharge of gas mixture of N_2 and helium.

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Synthesis of ZnO micro-spheres by the chemical vapor deposition(CVD)

정승환, 이상국

부산대 화학과

We were synthesized the ZnO micro-spheres by the chemical vapor deposition(CVD). The Si was used as a substrate and the mixture of ZnO/graphite powders was a precursor of ZnO micro-spheres. The precursor was loaded in the central region of the quartz tube furnace and Si substrate was placed downstream. Ar gas was introduced into the tube as a carrier gas. Under the atmospheric pressure, the precursor and the substrate was situated different temperature zone. After the reaction was terminated, a twinkling mixture of white and yellow products were obtained. We used scanning electron microscopy(SEM), high-resolution transmission electron microscopy(TEM), energy dispersive spectroscopy(EDS), x-ray photoelectron pectroscopy(XPS), photoluminescence(PL) to observed the morphology and structure of deposited materials.

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Observation of Vibronic Emission Spectra of jet-cooled o-Fluorobenzyl Radical

윤영욱, 이상국

부산대 화학과

We report the observation of jet-cooled o-fluorobenzyl radical in a corona discharge.Ther radical was generated and vibronically excited from the corona discharge of o-fluorotoluene seeded in a large amount of inert carrier gas by employing a pinhole type glass nozzle in a corona excited supersonic expansion. The vibronic emission spectra of the o-fluorobenzyl radical has been recorded with a long-path monochromator in the visible region. The vibrational mode frequencies in the ground electronic state were determined by comparison with those of o-fluorotoluene as well as those from an ab initio calculation.

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Field emission and secondary electron characteristics from α-Fe_2O_3 and TiO_2 coated α-Fe_2O_3 nanoparticles

신민경, *이휘건

*한양대 자연과학대학 화학과 *한양대 화학과*

α-Fe_2O_3 and TiO_2 coated α-Fe_2O_3 nanoparticles were formed by the chemical synthesis. The diameter of the rhombohedral structure of the α-Fe_2O_3 and TiO_2 coated α-Fe_2O_3 nanoparticles were about 80-100nm.The field emission properties were studied in a vacuum system. The Secondary electron emission measurement of primary current(I_p) and the scattered secondary electron(I_s), we calculated δ from the equation $\delta = I_s/I_p$. The following X-ray diffraction(XRD), Transmission electron microscopy(TEM) and SEM scanning electron microscopy(SEM) are used to characterize nanoparticles structural features.

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Molecular Dynamics for the Surface Deposition of Carbon Nanotube via Collision

Saha Leton Chandra, Mian Shabeer Ahmad, 김효정, Saha Joyanta Kumar, *장준경

*부산대 나노융합기술학과 *부산대 나노소재공학과*

We report a molecular dynamics simulation of a carbon nanotube deposited on a surface through collision. We demonstrate that the CNT forms a stable pillar structure on a silicon surface. Once the tube end of the CNT hits the surface at impact, the CNT finally stands upright regardless of its initial orientation. It is remarkable that the CNT reorients its axis spontaneously by an angle as large as 75º. The sputtering of silicon atoms together with the extensive fragmentation of CNT was observed for a high energy collision. The relaxation timescales were estimated for the structure and energy of the CNT excited by collision. The CNT relaxes its structure within 1 ps but its energy relaxation takes almost 10 ps. These results present an interesting implication for the alignment of CNTs on a surface through controlled collision, such as a molecular beam experiment.

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Comparative Study of Catechol and Water Adhesion on Silica Surfaces

Mian Shabeer Ahmad, Saha Leton Chandra, Matin Mohammad Abdul, 김효정, *장준경

*부산대 나노융합기술학과 *부산대 나노정보소재공학과*

Catechol (1, 2-dihydroxybenzene) functionality of marine mussels is speculated to be responsible for its strong and versatile adhesion on various wet surfaces. To enlighten the features of this adhesion, we performed a periodic density functional theory calculation for catechol adsorption on silica surfaces. We obtained its binding energy and geometry on two representative hydroxylated surfaces of cristobalite, which mimic amorphous silica. Catechol strongly adhered to both surfaces by making three or four hydrogen bonds. Catechol achieved versatility in adhesion via torsion of its hydroxyls. The binding energy of catechol, which amounts to 14kcal/mol, was larger than that of water, irrespective of the surface. The hydroxyls of catechol, not the phenylene ring, dominated its adhesion

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Lanthanide ion-doped upconverting nanoparticles (UCNPs) for real-time live-cell imaging

남상환, *배윤미, **박용일, **김정현, *최준식, ***이강택, **현택환, ****서영덕

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We employed lanthanide ion-doped upconverting nanoparticles (UCNPs) as the probe for real-time live-cell imaging. The luminescence of UCNPs upon NIR (980 nm) excitation lies in the visible range. Owing to the NIR excitation, the luminescence images were free of autofluorescent background from cellular environment, and the cells were not significantly damaged under long-time continuous illumination with high power density of the laser (~3 kW/cm^2). We could visualize the movement of the vesicles which encapsulated UCNPs in real time and the image data were analyzed by single particle tracking technique. Interestingly, the directed motions of the vesicles with the velocity of a few μm/s were frequently observed indicating that the UCNPs were actively transported by motor proteins, such as dynein or kinesin, moving along the microtubules.

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Live-cell imaging with upconverting nanoparticles: the long-term intracellular pathway of nanoparticles

배윤미, *남상환, **박용일, **김정현, 최준식, *이강택, **현택환, *서영덕

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Imaging nanoparticles in live cells provides deep insights into the interactions between nanomaterials and biological systems at the molecular and cellular level. The information thus obtained is crucial for designing efficient diagnostic and therapeutic strategies based on nanomaterials. We investigated the cellular uptake of newly developed upconverting nanoparticles (UCNPs), which emit visible photons upon near-infrared (NIR) excitation at 980 nm through two-photon upconversion process. Owing to the photostability of the particles and non-invasiveness of NIR excitation, we could monitor the cellular uptake process for a long period of time. UCNPs were generally internalized through endocytosis, accumulated at the perinuclear regions, and eventually discarded from the cells through exocytosis. The particles were found to be transported in the cytoplasm by microtubule-dependent motor proteins, which was supported by inhibition studies using a microtubule-disrupting drug.

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Simplistic Model for the Growth of a Monolayer in Dip Pen Nanolithography

김효정, *장지혜, *장준경

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Using a simple random-walk (RW) method, we simulated a monolayer growth in dip pen nanolithography (DPN). In the RW model, the process of monolayer growth is a combination of hopping down and serial pushing of molecules deposited from the tip. Applying the concept of directional coherence in pushing, our RW model quantitatively reproduces a molecular dynamics (MD) simulation for the DPN of nonpolar molecules on goldlike surfaces. It indicates that the pushing mechanism accurately explains the molecular motions in MD.

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Improved method for stabilization of TiO_2 nanoparticle suspension

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Stabilized nanoparticle suspension with high concentration is needed for the study of nanomaterial interaction with living bodies or physicochemical property characterization. We have developed the preparation method of stabilized TiO_2nanoparticle (NP)suspension without the addition of surfactant molecules. UV/Vis absorption spectrum, DLS (dynamic light scattering) size and zeta potential were measured to observe the property of TiO_2 NPs in suspension. The measurements were performed at various pH conditions and TiO_2 concentrations. By adjusting the pH of suspension with NaOH or HCl, we could obtain a stable TiO_2 NP suspension exhibiting maximal UV absorption with DLS size of ~ 200 nm when the concentration of TiO_2 was 3.7 mg/mL and suspension pH was 10. Since the addition of TiO_2 NPs into distilled water changes pH of the suspension, pH buffer solutions composed of acetate, phosphate or carbonate ions have been used as the solvents for the TiO_2 NP suspension. The maximum concentration of TiO_2 NPs in suspension could be increased by four and sixteen fold in sodium carbonate and phosphate buffer, respectively, compared with that in distilled water. The stability of suspension depending on the buffer ion concentration and pH was also tested by using DLS and UV/Vis absorption spectroscopy.

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Structure and Intramolecular Proton Transfer of Alanine Radical Cation

이갑용, *송영대, **권혁재

*대구가톨릭대 생명화학과 *경운대 한방자원학부 **대구가톨릭대 화학과*

The structure of the four lowest conformers of alanine, as well as their radical cations and the effect of ionization on the intramolecular proton transfer process have been studied using density functional and MP2 methods. The energy ordering for the radical cations of alanine differ from the corresponding neutral conformers. This result due to the changes in the basic and acid character of the NH_2 group upon ionization. Ionization favors the intramolecular proton transfer process that induces radical cation structure, [NH_3^+-$CHCH_3$-COO•]. For the proton transfer process the enegy barrier is observed to be about 6 kcal/mol.

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Investigation of the nanoenvironment and dynamics of single molecules in trehalose glass

박민규, 정병서

인천대 화학과

Trehalose, a nonreducing disaccharide of glucose, provides an interesting medium for biological applications due to its ability to stabilize proteins. Fluorescence from single fluorophore molecules was recorded as a function of time using single-molecule fluorescence microscopy, and the temporal fluorescence emission characteristics were analyzed to extract information on dynamical features and interactions of single molecules in trehalose glass films. In particular, correlations between the fluorescence fluctuations observed and trehalose content and hydration of sugar glasses were investigated. Comparisons were also made with the results observed in poly(vinyl alcohol), hydrophilic polymer film.

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Raman Spectroscopy Study of UV-Oxidized Graphene

안광현, 류순민

경희대 응용화학과

Graphene has drawn a great interest for its potential application in future electronics. Since graphene supported on a solid substrate is generally observed to be rippled on the nanometer scale, the influence of the structural deformation on its various properties is an important issue to be resolved. In this study, chemical activity of rippled graphene has been investigated by Raman spectroscopy. Nanometer scale corrugation was induced by thermal treatment exploiting differential thermal expansion between graphene and Si substrates. Oxygen atoms generated by UV photolysis of oxygen molecules were used as reactants, which attack the basal plane of graphene to form structural defects. The degree of the reaction was quantified by the disorder-related Raman D band and charge doping caused by the oxidation was monitored by Raman G and 2D bands.

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Raman Spectroscopy Study of Graphene on Atomically Flat Boron Nitride

송지은, 고택영, 류순민

경희대 응용화학과

Graphene, a single layer of graphite, has attracted significant research interest since its first isolation from graphite. Interactions between graphene and amorphous substrate like SiO_2/Si have been shown to limit charge mobility and mediate spontaneous hole doping in the ambient conditions. In this study, we have investigated environmental charge doping in graphene supported on hexagonal boron nitride, atomically flat insulating substrates. The layered composite samples were prepared by transferring graphene onto cleaved boron nitride flakes supported on SiO_2/Si substrates. Atomic force microscopy and Raman spectroscopy have been exploited to unravel the morphology of graphene and its interaction with the underlying substrates.

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Thermal Oxidation of Atomically Flat Graphene Supported on Mica

고택영, 심지혜, 류순민

경희대 응용화학과

Graphene has many fascinating material properties such as high electron mobility, high optical transparency, excellent thermal conductivity, superior Young's modulus, etc. Several studies have recently found that single-layer graphene is chemically more reactive than few-layer graphene. In this study, we have investigated the influence of structural deformation in graphene on its chemical reactivity. Thermal oxidation behavior of atomically flat graphene on mica substrates were studied by atomic force microscopy and Raman spectroscopy compared to graphene on SiO_2/Si substrates which cause finite roughness. Notably, oxidation of single-layer graphene proceeds more slowly on mica than SiO_2/Si. Detailed analysis led to a conclusion that deformation along the out-of-plane direction enhances reactivity of graphene.

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Charge Doping in Graphene on Highly Polar Mica

심지혜, 류순민

경희대 응용화학과

Graphene, one single atomic layer of graphite, has attracted extensive attention in various research fields since its first isolation from graphite. Its unique electronic structure and properties render graphene a fascinating material for various applications such as chemical sensors, transparent electrodes and field-effect transistors (FETs). Here, we present a study on charge doping and morphology of graphene supported on atomically flat and highly polar mica substrates. Ultra-flat single-layer graphene was prepared by micro-exfoliation of graphite followed by deposition on cleaved mica substrates at high (~50%) and low (

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The effect of nanoindentation on intermolecular fluorescence energy transfer

지아영

이화여대 화학나노과학부

Various nanoscopic sensors are based on stimulus-response systems in which stimuli may include thermal, chemical, electrical, optical, or mechanical means. Among these, mechanical sensors have been the least investigated, despite their great potential. We report the influence of mechanical deformation on the fluorescence resonance energy transfer (FRET) process, by using the Rhodamine 123 (R123) as a donor and azulene as an acceptor for FRET. For deformation-induced FRET, a flat indenter tip was used to press an elastomeric polymer and the fluorescence lifetime of the donor was measured in the presence of acceptors with respect to the indentation depth. Based on the FRET efficiency obtained in such a mechanoresponsive system, we have observed a significant FRET enhancement when the polymer matrix was structurally deformed.

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Raman Spectroscopy Study of Crystallographically Oriented Graphene Edges

박민규, 류순민

경희대 응용화학과

Theory predicts very different properties for graphene nano-objects terminated with zigzag and armchair edges. Controlling such edges, however, has been far from experimental realization until a recent claim of formation of zigzag-terminated graphene edges by carbothermal reaction. In this study, we have investigated structural details of crystallographically oriented edges reproduced based on the previous work. The morphology of carbothermally etched graphene edges was studied by atomic force microscopy. Raman spectroscopy served as a valuable tool to monitor the formation of zigzag edges.

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Effect of the adsorption solvents and electrolyte additives on the photovoltaic performances of Zn porphyrin analogues

Mannix Balanay, 이미정, 이상희, 김동희

군산대 화학과

Two Zn porphyrin dyes, cyano-3-(2'-5',10',15',20'-tetraphenylporphyrinato zinc(II)yl)-acrylic acid (ZCA-1) and cyano-3-(2'-5',10',15',20'-tetratolylporphyrinato zinc(II)yl)-acrylic acid (KS-4) were synthesized and characterized by various spectroscopic techniques. A density functional theory based on the Coulomb attenuated method was used to depict the charge-transfer excitation energies. The DFT calculations also show that the key molecular orbitals of both porphyrins are extended onto the substituent by π-conjugation. The addition of the methyl group at the para-position of the meso-positioned phenyl rings in KS-4 analogue resulted in a narrower band gap compared to ZCA-1. The polarity of the solvent used in the sensitization of the dye into the semiconductor plays a vital role in the photovoltaic performance of the porphyin-based dye. The use of a very low polarity solvent (Toluene) in the sensitization process produced almost twice the efficiency than using a moderately polar solvent (THF). The photovoltaic performance of the porphyrin analogues were also assessed with the use of different electrolyte composition.

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산화 아연 단결정 표면 에서의 수소 반응에 대한 연구: 비교연구

Probir Chandra Roy, 김창민

경북대 화학과

The interaction of hydrogen and ZnO single crystal surfaces, ZnO(000-1), ZnO(10-10) and ZnO(11-20), has been investigated using temperature programmed desorption (TPD) and low energy electron diffraction (LEED) techniques. When the ZnO single crystal surfaces are exposed to atomic hydrogen, hydrogen is adsorbed on the surfaces. As the surface are saturated with adsorbed hydrogen, bulk diffusion of hydrogen takes place. The existence of surface and bulk hydrogen has been confirmed by using X-ray photoelectron spectroscopy (XPS). Diffusion of hydrogen into the ZnO bulk is an activated process. Activation energies of the ZnO single crystal surfaces have been estimated. We will report the effect of the structure on desorption of hydrogen.

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Spatial organization of the flow of Green fluorescent protein in Escherichia coli by Fluorescence Lifetime Imaging Microscopy(FLIM)

이길용, 김은철, 김희태, 서갑석, 안태규

성균관대 에너지과학과

The green fluorescent protein (GFP) has become an invaluable marker for monitoring protein localization and gene expression in vivo. We imaged mixed populations of Escherichia coli expressing EGFP by Fluorescence Lifetime imaging Microscopy(FLIM) Our goal is to visualize and quantify the spatial distribution of specific expressed EGFP under conditions in which protein is synthesized and degraded normally. Our findings show that EGFPs spatially diffuse after synthesis in E.coli. This work has important implications for cellular physiology and for understanding of protein diffusion in E. coli.

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Structures and properties of cyclic thiophenederivatives. A Theoretical Study

최호준, *구인선, *박종근, *송상순

*경상대 화학과 *경상대 화학교육과*

Cyclic thiophene derivatives (n=6~38, even only) and its CnT (n=8~28) complexs with polycyclic aromatic hydrocarbons (PAHs, An, n=1~6), fullerenes, and carbon nanotubes are optimized at the HF//3-21G*/6-31G* and B3LYP//LANL2DZ levels. Geometrical structures, bond lengths, dihedral angles, and HOMO-LUMO gaps of neutral, dication, tetracation, and möbius structural derivatives have been analyzed. In neutral cyclic thiophenes, the structures of (n=6~8) are distorted and the structures of (n=10~14) are planar. With increasing n (n>14), the structures varied to the bend type.

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Sintering behavior of copper nanoparticles

유은결, 김상호, PIAO LONGHAI

공주대 화학과

Developing a low cost printing material that can replace silver for the formation of a conducting pattern is an important issue in printed electronics. Among many materials, copper seems to be a reasonable choice to replace a silver material because of its high electric conductivity and low price. However, there exist one huge problem to be solved in order to employ copper as a printable electrode material: the oxidation of copper during the sintering process. In this study, the sintering behavior of copper nanoparticles was examined by varying the sintering temperature, time and the environment. Scanning electron microscope (SEM), and tunneling electron microscope (TEM) analysis revealed the morphological change during the sintering process. X-ray diffraction (XRD) analysis showed the crystallinity, composition and the grain size of copper depend on the various sintering conditions and which eventually affect the electric properties of the electrode.

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Detection of duplex cancer marker genes using surface-enhanced Raman scattering (SERS)-based optofluidic sensor

최남현, 추유진, 이남우르레흐만, 이문권, 주재범

한양대 바이오나노공학과

We present the application of a surface enhanced Raman scattering (SERS) method for a sensitive detection of duplex cancer marker genes in a gradient microfluidic channel. This technology does not need either an immobilization procedure or PCR amplification, which are essential for a DNA microarray. This SERS-based optofluidic sensing technique also provides a rapid and sensitive detection of DNA markers. Herein, a gradient microfluidic channel was used to automatically generate different mixing ratios of duplex DNA samples. By using this, a tedious manual mixing process is eliminated and a fast and sensitive DNA analysis could be achieved under flowing conditions. BRCA1 and BAX were used as target genes. BRCA1 is a gene over-expressed in breast cancer cells, and BAX is known to be closely related with its apoptosis. In this presentation, the application of SERS-based optofluidic sensor for highly sensitive cancer gene (BRCA1 and BAX) diagnostics will be introduced.

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Adhesion promoter for silver nano-ink

홍준의, 김상호, **PIAO LONGHAI**

공주대 화학과

Silver nano-ink has been widely studied and applied in many printable devices such as radio frequency identification (RFID), printed circuit board (PCB), thin film transistor liquid crystal display (TFT LCD) and so on. Silver nano-ink, being heat-treated at low temperature (4B (Cross Cut test, ASTM class). Through this study, the printed electrode using silver nano-ink showed excellent adhesion and flexibility as well as good electric conductivity.

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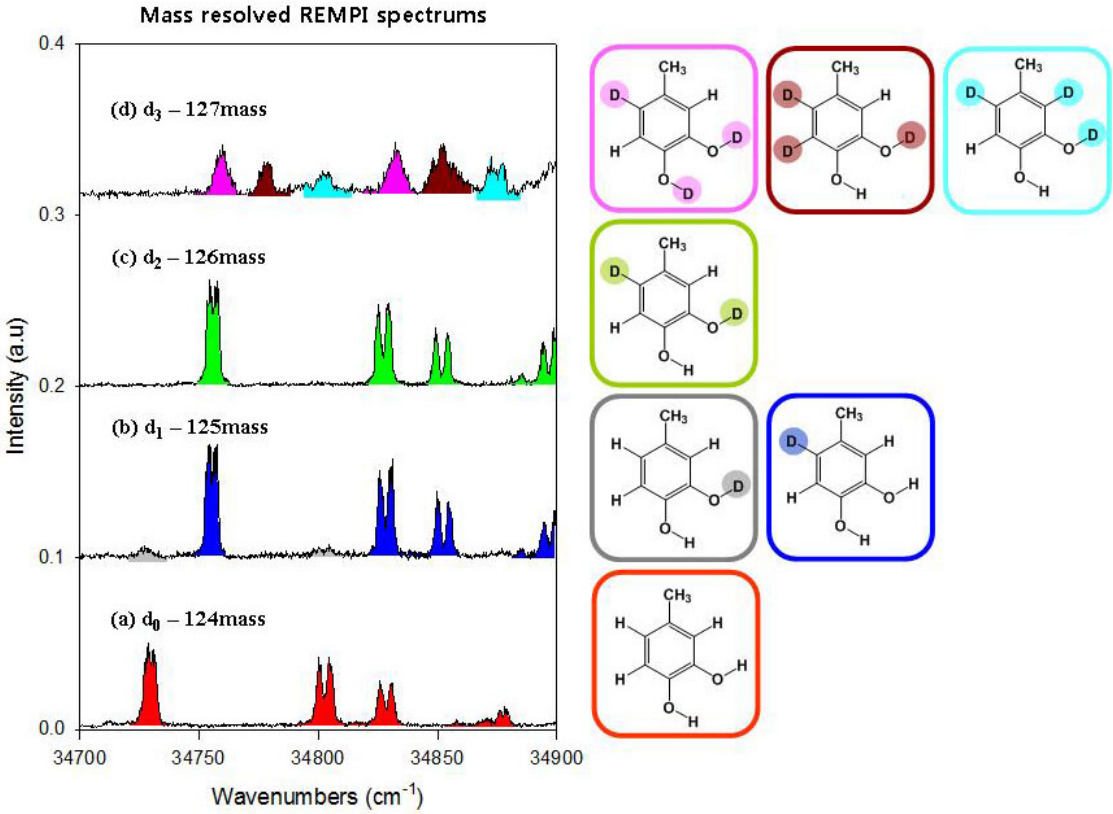
Theoretical and spectroscopic studies of the deuterated species of 4-methylcatechol

장성우, 곽현태, *임상규, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We previously reported the spectroscopic studies of the deuterated species of supersonically cooled 4-methylcatechol using the REMPI spectroscopy and theoretical calculations(ab initio and DFT). The REMPI spectra of partially deuterated d_1-, d_2-, d_3-4-methylcatechol were measured and the relative shifts of the electronic band origins(the $S_0 \rightarrow S_1$ transition) were interpreted by theoretical calculations performed using the complete active space self-consistent field(CASSCF) theory with the 6-31G(d,p) basis set. The intermediates or transition states of the deuterated species produced from electrophilic substitution and tautomerization (hydrogen/deuterium exchange) were calculated using the ab initio and DFT methods applying the solvent effect. The results were discussed in comparison with the hydrogen/deuterium exchange reactions of catechol(1,2-dihydroxybenzene) and resorcinol(1,3-dihydroxybenzene).



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Photoinduced Isomerization Study of Resveratrol

강준희, *양일승, **김성근

*서울대 생물물리 및 화학생물학과 *서울대 화학부 **서울대 화학부 & 생물물리 및 화학생물학과*

Resveratrol is a phytochemical compound naturally found in various plant species, most notably in grapes and berries. Much interest has been drawn to this compound in the last few decades because of its anti-oxidant, anti-inflammatory, and anti-tumorigenic effects. Resveratrol exists as either the trans- or cis-isomer, which easily undergoes isomerization by exposure to sunlight or UV radiation. The trans-isomer exists in natural products while the cis-isomer is mostly found in grape wines, with both isomers reported to show similar physiological effectiveness. Despite the numerous studies on the biological activities of resveratrol, the photodynamical properties are poorly understood. We employed transient absorption and stimulated Raman spectroscopy to elucidate the photodynamical properties of resveratrol.

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Mechanisms for selective S-S and C-S bond cleavage in radical driven free radical initiated peptide sequencing mass spectrometry

이윤진, 문봉진, 오한빈

서강대 화학과

Previously, we have shown that TEMPO-FRIPS method is useful for peptide sequencing and that it shows a fragmentation pattern totally different from that of commonly used CID. In the present study, we applied this method to investigate the plausibility of disulfide bond cleavage, which may facilitate the peptide mass spectrometry analysis by skipping disulfide bond reduction/alkylation procedure in bottom-up mass spectrometry analysis. We observed that five different peptides with a disulfide bonds, three cyclic peptides and two linear peptides, are commonly cleaved at the S-S and C-S bond positions. The generated free radical resulted in fragmentations in both the S-S bond and backbone bond. In this poster, we will show the detailed mechanistic pathway of disulfide bond cleavage.

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Single-molecule FRET with Alternating Laser Excitation

최윤미, 정지원, *임영빈, **이남기, ***김성근

*서울대 화학부 *서울대 생물물리 및 화학생물 **포항공과대 시스템생명공학부/물리학 ***서울대 화학부, 서울대 생물물리 및 화학생물학과*

We studied intracellular membrane fusion mediated by soluble N-ethylmaleimide-sensitive factor attachment protein receptors (SNAREs) in vitro by examining the fusion of SNARE-laden vesicles at the ensemble level. The SNARE-driven membrane fusion was also investigated at the single-molecule level by monitoring the mixing of lipids labeled with DiI and DiD using alternating-laser excitation(ALEX)-FRET. The necessity for the single-molecule measurement was confirmed to distinguish vesicle fusion from vesicle aggregation. We demonstrated by employing fluorescence fusion assay that SNAP-25 protein is essential for membrane fusion between vesicles with v-SNARE and t-SNARE.

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Charge Transfer between Graphene and a Strong Electron Acceptor, Tetrafluorotetracyanoquinodimethane (F4-TCNQ)

이지은, 김선호, 양성익, 류순민

경희대 응용화학과

Graphene, a single atomic layer of sp2-bonded carbon, shows substantial potential for various applications. Chemical manipulation of its electronic properties will be of great importance. In this study, we have investigated interaction between graphene and organic molecular layer of tetrafluorotetracyanoquinodimethane (F4-TCNQ), a strong electron acceptor. F4-TCNQ films of varying thickness were evaporated onto graphene mechanically exfoliated on SiO2/Si substrates. Raman spectroscopy study revealed significant hole-doping in graphene caused by electron transfer to F4-TCNQ. Growth of the films on graphene was also studied by atomic force microscopy.

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Synthesis of Au-Cu2S Nanocrystals and Their Visible-Light-Driven Photocatalytic Activity

김윤희, 박기영, 장동명, 박정희

고려대 소재화학과

Au-Cu2S core-shell NPs were synthesized for the first time using the in-situ solvothermal growth of Cu2S on Au. The average sizes of the Au-Cu2S and Au core NPs were 7 and 3 nm, respectively. The photocatalytic degradation of methylene blue was achieved using the free Cu2S and Au-Cu2S under visible light irradiation. The incorporation of the Au core into the NPs significantly decreases their efficiency to 70 %. The comprehensive data analysis suggests the excellent photocatalytic reduction activity of the Cu2S NPs toward the generation of H2O2, which leads to the oxidative degradation of methylene blue. Their photocatalytic reduction power would be suppressed as the Au core withdraws the electrons from the Cu2S shell.

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A High-Efficiency Surface-Enhanced Raman Scattering SubstrateBased on ZnO Nanowires Array Decorated with Silver Nanoparticles and Gold Nanoparticles

백선영

고려대 소재화학과

Surface-enhanced Raman spectroscopy (SERS) has attracted intense interest since 1977, beacause SERS has been extensively utilized to detect chemical and biological molecules. We introduce a unique surface-enhanced Raman scattering (SERS) substrates, which is made of nanoarrays comprising zinc oxide nanowires (ZnO NWs) decorated with silver nanoparticles (AgNPs) and gold nanoparticles (AuNPs). The ZnO NWs arrays were produced through hydrothermal method, and then deposited with the AgNPs and AuNPs using SILAR (Successive Ionic Layer Adsorption and Reaction) method. The sizes were controlled in the range of 5-30 nm The substrates exhibited strong surface-enhanced effect in Raman. The results suggest that the deposition of noble metal NPs effectively enhances field enhancement by localized surface plasmons, which promise excellent new typed nanostructures for the SERS.

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Solvothermal synthesis of CdSe/ZnS nanoparticles using ionic liquids as capping ligands

송윤미, *장동명, *박기영, *박정희, **차은희

*고려대 소재화학과 태양에너지소재 *고려대 소재화학과 **호서대 화학*

Ionic liquids are room-temperature molten salts, composed of organic mostly of organic ions that may undergo almost unlimited structural variation. We approach the new aspects of ionic liquids in applications where the semiconductor nanoparticles used as sensitizers of solar cells. We studied the effects of ionic liquids as capping ligand and/or solvent, on the morphology and phase of the CdSe/ZnS nanoparticles. Colloidal CdSe/ZnS nanoparticles were synthesized using a series of imidazolium ionic liquids; 1-R-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([RMIM][TFSI]), where R = ethyl ([EMIM]), butyl ([BMIM]), hexyl ([HMIM]), octyl ([OMIM]). The average size of nanoparticles was 8~9 nm, and both zinc-blende and wurtzite phase was produced. We also synthesized the nanoparticles using a mixture of trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide ([P6,6,6,14][TFSI]) and octadecene (ODE). The CdSe/ZnS nanoparticles have a smaller size (5.5 nm) than that synthesized using imidazolium, and with a controlled phase from zinc-blende to wurtzite by increasing the volume ratio of [P6,6,6,14][TFSI]. For the first time, the phase and size control of the CdSe/ZnS nanoparticles was successfully demonstrated using those ionic liquids.

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Synthesis of TiO2/GaP core-shell nanocables for Photoelectrochemical water splitting

강준하, 박정희

고려대 소재화학과

High-density TiO2/GaP core-shell nanotube arrays were synthesized using electrochemical method, and TiO2 nanowires were synthesized using thermal oxidation of Ti foils. The diameter of TiO2 nanotube was controlled using the growth condition. The GaP layers were deposited on the pre-grown TiO2 nanotubes(anatase) and TiO2 nanowires(rutile), using vapor transport method. The products are analyzed by using SEM, XRD, and TEM.

THE KOREAN CHEMICAL SOCIETY

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Synthesis and optical properties of CdSSe Nanowires and TiO2@CdSSe Nanocables using vapor transport method

성태광

고려대 소재화학과

Ternary alloy CdSSe nanowires and TiO2@CdSSe nanocables were successfully grown through a thermal evaporation route using Au catalyst and TiO2 substrate. High-resolution transmission electron microscopy, energy dispersive x-ray spectra and x-ray diffraction showed that both the nanowires and the nanocables have high-quality single-crystalline,and their compositions can be determined as CdS and CdS0.85Se0.15,and CdS0.75Se0.25 and CdS0.6Se0.4 and CdS0.2Se0.8 and CdSe respectively. TiO2@CdSSe nanocables compositionscan be determined as CdS, and CdS0.75Se0.25 and CdS0.8Se0.2 and CdSe respectively.The photoluminescence measurements showed very strong band-edge emission for samples, which further demonstrates the single-crystal nature of the as-obtained CdSSe alloys. This finding may be extended for fabricating other composition-tunable 1D ternary alloy nanostructures

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"Orbital Asymmetry" and Orbital Energy Reordering inElectron Attachment to X-benzene (X=BrCl, IBr, ICl)

손태일, 김남두, 이상학, *김성근

*서울대 화학부 *서울대 화학부&생물물리 및 화학생물학과*

The electron-binding properties of X-benzene (X=BrCl, IBr, ICl) have been investigated by using photoelectron spectroscopy and ab initio calculations. Full molecular orbital calculations of neutral and the corresponding anion have been performed by the DFT and MP2 methods. Photoelectron spectra were obtained at 355 nm to characterize the electronic structure of anionic X-benzenes. Vertical detachment energies of X-benzenes obtained by ab initio calculations agree well with the experimental values. Interestingly, when the electron is attached to X-benzene, most of its charge is localized in the atom that has a smaller electronegativity value, in accord with what is known as "orbital asymmetry". We found that the molecular orbitals undergo considerable reordering in energy as the electron approaches X-benzene.

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Gold(Au) nanocrystals and their Au_2S nanocrystals 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-Au_2S 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 Au_2S 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 Au, Ag, Pt NCs and their Au_2S NCs 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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Competitive activation of C-F and C-H bonds in reactions of Os^+ with CH_3F: A theoretical study

홍기룡, 김태규

부산대 화학과

The gas phase reaction of activation C-H and C-F bonds of CH_3F by Os^+ (6D and 4F) ion has been studied using density functional theory (DFT) to understand about reaction mechanisms and pathways. The primary reaction channels of the reaction of Os^+ with CH_3F are H_2 elimination and HF elimination and both reaction pathways are exothermic. The molecular structures of intermediates and transition states were optimized at the B3LYP level for both H_2 and HF elimination pathways. All transition states were identified by using the intrinsic reaction coordinate method. According to the revealed mechanisms and the calculated potential energy surfaces, H_2 elimination is the most favorable product channel which has a smallest barrier height. The results of this study were compared with the available experimental observations.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Competitive activation of C=O and C-F bonds in Reaction of Ti^+ with CF_3COCH_3: Experimental and Theoretical investigation

홍기룡, 폴다바브라타, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

The gas phase investigation of ion-molecule reactions within $Ti^+(CF_3COCH_3)_n$ clusters has been performed by using laser ablation-molecular beam/reflextron time-of-flight mass spectrometry. The primary reaction channels of the reactions of Ti^+ with CF_3COCH_3 are TiF_2^+ and TiO^+ formation. These ionic clusters were demonstrated via competitive C-F and C=O bond activation, respectively. Theoretical investigation was performed to present about the geometrical optimization for reaction species and reaction pathways. The calculation results also have been found both TiF_2^+ and TiO^+ formation channels. Further the potential energy surfaces of doublet and quartet spin states about both reaction channels are presented. The computational results show good agreements with the experimental findings.

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Synthesis and Characterization of Cobalt Selenide Nanowires

고경문, 김태규

부산대 화학과

In our present study, we have successfully synthesized the cobalt selenide (CoSe) nanowires by a chemical vapor deposition (CVD) on Au-coated Si(100) substrate. The growth on Au-coated Si(100) substrate was founded through vapor-liquid-solid (VLS) mechanism where cobalt chloride ($CoCl_2$) and selenium (Se)-graphite mixture were used as precursors. Graphites have been used for the purpose of control of the vaporization rate of selenium (Se) during the experiment. Scanning electron microscopy (SEM) and Transmission Electron Microscopy (TEM) measurements revealed that the CoSe nanowires were 60-100 nm in diameter and 10-20 μm in length. The Energy Dispersive X-ray Spectroscopy (EDS) data indicate that the growth of CoSe nanowires shows homogeneous character. The synthesized nanowires were also investigated by X-ray diffraction (XRD) method to elucidate the detail structure of CoSe nanowires.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Membrane Introduction Mass Spectrometry: Interfacing Nafion Membrane Inlet with Portable Time-of-Flight Mass Spectrometer

김현국, 김태규

부산대 화학과

Membrane introduction mass spectrometry (MIMS) is one of the simplest, most efficient, and most sensitive techniques for the purpose of on-line/on-sites analysis of volatile organic compounds (VOCs) and other analytes. The working principles of MIMS lies in the fact that VOCs selectively permeates through hydrophobic membrane such as such as polydimethylsiloxane(PDMS), also known as silicone, much more quickly than water and other polar substances. In this work, we used the Nafion membrane which is one of hydrophilic membrane, as a membrane interface in the MIMS method for comparison with silicone membrane based MIMS. We analyze low molecular weight alcohol and other polar compounds and measured the response times, limits of detection and diffusion coefficient for each compound. Finally we compared our results with silicone membrane based MIMS method and discussed potential uses of hydrophilic membrane in MIMS.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Ni-doped Ge Nanowires Properties Synthesized by Chemical Vapor Deposition

이우영, *김태규

*부산대 물리화학 *부산대 화학과*

Ni-doped Ge nanowires have synthesized via chemical vapor deposition (CVD) method. Ni is a potential kind of magnetic transition metal and Ge has low band gap, high hole electron mobilites and large exciton radius as semiconductors. Homogeneous Ni-doped Ge nanowires are grown onto the Au-coated Si substrate. The particle morphology and structure were characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Ni-doped Ge nanowires are reacted for 20 min that resulted in high yield of homogeneous growth of diameter 60 ~ 120 nm and length up to several tens of microns. The Ni concentration (in at. %) as processed by energy dispersive x-ray (EDS) technique is about 5 %. The structure, optic and magnetic properties of Ni-doped Ge nanowires were investigated by X-ay diffraction (XRD) and photoluminescence (PL). The presence of Ni in Ge environment of chemical states is detected by X-ray photoelectron spectroscopy (XPS). The crystallization characteristic of samples is analyzed by Raman spectroscopy. Properties of Ni-doped Ge nanowire have been discussed by a comparison with undoped-Ge nanowires.

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Gas Phase Ion-Molecule Reaction within $Fe^+(C_2H_5OC_2H_5)_n$ Heteroclusters

폴다바브라타, 홍기룡, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

The intracluster ion-molecule reaction of $Fe^+(C_2H_5OC_2H_5)_n$ clusters were investigated by using a laser ablation-molecular beam/reflectron time-of-flight mass spectrometer. The mass spectrum obtained from the reaction of Fe^+ with diethylether exhibits three major sequences of cluster ions with the formula (i) $Fe^+(C_2H_5O)(C_2H_5OC_2H_5)_n$, (ii) $Fe^+(C_2H_5OH)(C_2H_5OC_2H_5)_n$ and (iii) $Fe^+(C_2H_4)(C_2H_5OC_2H_5)_n$.The formation mechanism of $Fe^+(C_2H_5O)(C_2H_5OC_2H_5)_n$, $Fe^+(C_2H_5OH)(C_2H_5OC_2H_5)_n$ and $Fe^+(C_2H_4)(C_2H_5OC_2H_5)_n$sequences are demonstrated as plausible C-O bond activation followed by direct cleavage and intracluster rearrangement-competitive elimination mechanism, respectively. Simultaneously, the simple ion-molecule reaction product ($Fe^+((CH_3CHO))$ which is existed only in the low mass region, is attributed via C-O bond activation of solvated diethylether molecule, lead to β-H atom transfer and elimination of ethane. The H_2 elimination and hydrogen extraction are mainly originated from insertion of Fe^+ into the C-H bond. The formation mechanisms and reaction energetics for the observed primary heterocluster ions are discussed by using the density function calculation results.

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Effect of Substitution on Intracluster Ion-Molecule Reactions within $Ti^+(C_2H_5XC_2H_5)_n$ (X = O and S) Clusters

폴다바브라타, 홍기룡, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

We have investigated the dynamic insertion of Ti^+ ion within $Ti^+(C_2H_5XC_2H_5)_n$ (X = O and S) heteroclusters by using laser-ablation/supersonic beam expansion method. The mass spectra of $Ti^+(C_2H_5OC_2H_5)_n$ exhibit a major sequence of cluster ions with the formula $TiO^+(C_2H_5OC_2H_5)_n$, which is attributed due to the effective oxidation of $(C_2H_5OC_2H_5)_n$ molecule. The other two primary products, $Ti^+(C_2H_4O)(C_2H_5OC_2H_5)_n$ and $Ti^+(EtO)^+(C_2H_5OC_2H_5)_n$ in the entire the mass spectrum are originated from the intracluster rearrangement-elimination and the direct cleavage mechanism of unidirectional C-O bond activation, respectively. On the other hand, the sulfur substituted cluster ion, $Ti^+(C_2H_5SC_2H_5)_n$, shows strikingly different three major sequences of cluster series: (i) $Ti^+(CH_4)(C_2H_5SC_2H_5)_n$, (ii) $TiS^+(C_2H_5SC_2H_5)_n$, and (iii) $Ti^+(C_2H_4S)(C_2H_5SC_2H_5)_n$, The $Ti^+(CH_4)(C_2H_5SC_2H_5)_n$, $TiS^+(C_2H_5SC_2H_5)_n$, and $Ti^+(C_2H_4S)(C_2H_5SC_2H_5)_n$, clusters formation were exclusively dominated by the competitive insertion of Ti^+ into C-C and C-S bonds of $(C_2H_5SC_2H_5)$ molecule. The promising competitive product ion, $Ti^+(CH_4)(C_2H_5SC_2H_5)_n$, was demonstrated followed by α-H atom transfer and elimination of $HCSCH_2CH_3$ molecule. The sequential reactions of primary product ions for both systems are also observed and discussed.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Mechanistic Insights into Nickel-Catalyzed Hydroheteroarylation of Vinylarenes

GAO JIEYING, su zhishan, *이해황, *김찬경, **Ying Xue

*인하대 물리화학 *인하대 화학과 **College of Chemistry, Sichuan University, PR China*

The mechanisms of nickel-catalyzed hydroheteroarylation of vinylarenes were studied by use of computational techniques. Optimized structures for all of the stationary points in the gas phase were investigated using HF method. The SDD pseudopotential, along with its associated basis set, was used to describe the nickel centers, while the 3-21G basis set was used for the main group atoms C, O, N, and H. Three possible pathways in the title reaction were considered, involving the conventional oxidative addition (path A), carbon-assisted C-H bond activation (path B) and nitrogen-assisted C-H bond activation (path C). Our results indicate that for the C-H bond activation step (the first step), path A is more favorable than paths B and C in the gas phase.

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Theoretical Investigation on the Mechanism of Enantioselective Michael Addition of Malononitrile to Chalcones Catalyzed by Quinine–Al(OiPr)3 Complex

su zhishan, *이해황, *김찬경

*인하대 물리화학 *인하대 화학과*

The mechanism of enantioselective Michael addition of malononitrile to chalcones catalyzed by quinine–Al(OiPr)3 complex was investigated by DFT and ONIOM methods. The computational results indicated that the Al(III)-complex catalyzed reaction proceeded through a stepwise mechanism, and the step corresponding to the transfer of H atom from quinine unite to C atom of chalcone was predicted to be the rate-determing step. The steric hindrance of aromatic ring connected to carbonyl group of chalcone played an important role in controlling the stereoselectivity of reaction. The transition state with the lowest energy corresponded to the S-products, which was in agreement to the experimental observations.

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Time-resolved spectroscopic studies on electron flow systems

김은철, *김근돈, *유상동, 안태규

*성균관대 에너지과학과 *성균관대 생명과학과*

Photosynthetic light reactions in plant chloroplasts are suitable for spectroscopic (fluorescence) study because those undergo energy transfers from chlorophyll a to reaction center complexes. The fluorescence measurement using plant leaf organs has been developed and studied more than 30 years. Recent developments of fluorescence life-time imaging microscopy further enable to study time-resolved fluorescence (TRF) at a cellular level. However, it is still not so straight forward to acquire and interprete the data from intact leaf tissues, due to the interference of cell walls for fluorescence measurements. Thus, little is known for TRF by chlorophyll a, that is the key light energy absorbing pigment in plant chloroplasts. To explore energy transfer scheme during photosynthesis with TRF analysis, we have applied the protoplasting technique and isolated leaf mesophyll cells without cell walls. We then quantitatively measured transitions of chlorophyll a in plant cells before and aftertreatments of DCMU(diuron), which blocks the electron flow from Q_A to Q_B by displacing Q_B from its binding site. Abrupt increase of fluorescence lifetime was observed with the DCMU treatment indicating a slow decay rate of energy when the electron transfer from chlorophyll a to reaction center complexes was blocked(figure 1). We have, here by, proved the concept of photosynthetic energy transfer using TRF analysis with the manipulation of its electron flow by DCMU in plant cells.

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Electronic and Structural Dynamics in Solvated Transition Metal Complexes by Femtosecond Soft X-ray Spectroscopy

조하나, 홍기룡, 김태규

부산대 화학과

The knowledge of temporally varying valence electronic structures during ultrafast processes is vital in understanding the rearrangement of chemical bonds and their cooperative relationship with atomic position. For this purpose, ultrafast soft x-ray absorption spectroscopy of first-row transition metal complex at metal L-edge is appropriate for delivering detailed information on the evolution of electronic structure. Herein we report femtosecond soft x-ray spectroscopy of solvated Fe(II) complex for the first time. Our data provide detailed information on the nature of transition metal-ligand interactions followed by spin state transition. The results in this work demonstrate the feasibility and potential of femtosecond soft x-ray absorption spectroscopy to study ultrafast processes in liquid phase by probing dynamic changes in valence electron orbitals.

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Theoretical Study of M(CH6H6) cation (M: Ca, Zn, Cd, Hg, Yb) :DFT Study

서영선, *이지현, 이기학

*원광대 화학과 *원광대 생명나노화학과*

The thermochemistry structural chemistry and biochemistry of atomic cation-π interactions involving benzene have been receiving growing attention in recent years, particularly since benzene has become a prototype aromatic molecule in the study of cation-π interactions that determine the structures of bimolecular. We theoretically investigate the structures and binding characteristics of Metal cations (Ca+,Zn+,Cd+,Hg+,Yb+) interaction with benzene. Metal-benzene complexes were optimized using DFT calculations [Becke three parameters with the Lee-Yang-Parr functional (B3LYP)]. The basis set for benzene was used with the 6-311+g*. The pseudopotentials of transition metals were used with the Stuttgart RSC segmented/ECP.

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Molecular dynamics simulation study on ordered structure of ionic liquids in bucky gels

박상원, 정연준, *Hyung J. Kim

*서울대 화학부 *bDepartment of Chemistry, Carnegie Mellon University*

Upon mixing with ionic liquids (ILs) based on imidazolium ions, carbon nanotubes (CNTs) form physical gels, called "bucky gels"[1]. Their versatile properties, such as flexibility and electrical conductivity, can be adopted as electrochemical devices, for example, sensors, capacitors, and actuators. While experimental studies have given a conjecture that π-π stacking between the imidazole rings of the cations of ILs plays an important role on the gel formation, the molecular-level understanding of their structure has not been provided. In this study, we present a structure of bucky gel composed of CNTs in 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM]BF_4) obtained via molecular dynamics simulations. It is found that imidazole rings of cations in the first cylindrical solvation shell are mainly parallel to the CNT surface, indicating π-π stacking between the CNT and $[EMIM]^+$ ions, which is consistent with our previous study[2]. Molecular ordering of ILs between the CNTs is also investigated with respect to the radial direction in variation with separation of the CNTs, i.e., concentration of the CNTs. Further, we explore how temperature and the length of alkyl chains in the cation affect the ordered structure in bucky gels.

References

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2. Shim, Y.; Kim, H. J. *ACS Nano* 2009, 3, 1693.

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Numerical study on lowering of dynamic heterogeneity in supercooled liquids at spatially high dimensions

김소리, 정연준

서울대 화학부

We use kinetically constrained models to investigate a dimensional dependence of dynamic heterogeneity in supercooled liquid systems. Higher dimensional generalizations of Fredrickson-Andersen (FA) and East models are used as representative strong and fragile liquid systems. We first investigate how the breakdown of the Stokes-Einstein (SE) relation changes with the system dimensionality. The scaling $D \sim \tau^{-\xi}$ reveals that there is a weak violation of the SE relation at low temperature for strong liquid models with ξ becoming close to 1 as the dimensionality increases. However, for the East model and its higher dimensional versions, there is still significant Stokes-Einstein violation at d=4 and higher dimensions, although its extent weakens as d increases. Our result is consistent with recent molecular dynamics simulation studies performed on supercooled liquid systems. We further present other numerical results such as dynamic susceptibility to investigate the dimensional dependence of the heterogeneous dynamics in glass systems.

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Triplet state and phosphorescence of hole-transport layer (m-MTDATA) and its triplet exciton confinement

서주희, 한노수, 심형섭, 박승민, 송재규

경희대 화학과

Triplet state of 4,4′,4″-tris(3-methylphenylphenylamino)triphenylamine (m-MTDATA) and dynamics of the singlet and the triplet states were investigated to understand the confinement effect of m-MTDATA as host materials for a phosphorescent organic light-emitting diode. Time-resolved photoluminescence spectra revealed phosphorescence around 480 nm (2.58 eV). The time constant of the T1 state was 1.2 ′ s. The dynamics of delayed fluorescence was found to be closely related to that of phosphorescence. The triplet energy of a green phosphorescent sensitizer turned out to be well-confined in the m-MTDATA host, which suggested the application of m-MTDATA as possible host materials.

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Ultraviolet lasing in single ZnO nanowire at Room-temperature

심형섭, 한노수, 서주희, 박승민, *최명룡, 송재규

*경희대 화학과 *경상대 화학과*

ZnO is a well-known wide band-gap semiconductor suitable for blue optoelectronic applications. In particular, the lasing in ZnO nanowires due to photonic confinement effects has been widely studied. With the excitation of femtosecond laser pulses, the lasing action of ZnO nanowires prepared by chemical vaporization deposition methods was observed, because the excitation pulses were shorter than the duration time of lasing. The exotic lasing in nanowires was found as a function of the excitation intensity, where the peak wavelength of lasing was blue-shifted and another peak of the longitudinal modes appeared with the increase in the excitation intensity. The mechanism of the blue-shifted lasing and the appearance of the longitudinal modes were carefully investigated.

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나노 입자 분리를 위한 나노 세공을 가진 알루미늄판의 제조

소수정, 한종수

전남대 화학과

나노입자의 크기에 따른 분리는 나노입자 사용공정에서 매우 중요하지만 ultra filtration 외에 다른 방법이 발견되지 않고 있다. 나노 입자를 분리하는 또다른 방법으로 입자와 굴곡을 가진 표면간의 상호작용을 이용할 수 있을 것이라고 보고 본 연구에서는 20~80nm 의 굴곡내지 얕은 세공을 갖는 알루미늄판을 양극 산화로 형성하였다. 양극 산화에 사용된 산은 인산, 황산, 옥살산이었고, 전류밀도 1~10mA/cm2 였다. 표면 세공의 크기 그리고 나노크기 실리카 입자와 표면의 상호작용 형상을 SEM 으로 관찰하다.

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Matrix-free laser desorption/ionization on a flat surface

김신혜, 이애라, *송재용, 한상윤

*한국표준과학연구원 나노바이오융합연구단 *한국표준과학연구원 산업측정표준본부*

In this work, we demonstrate that matrix-free laser desorption/ionization is possible even on a flat surface without utilizing any nanostructure. It was demonstrated for ionizing various molecules with masses up to 1600 Da. Further surface derivatization greatly improved the ionization efficiency, providing the sensitivities of 0.01 fmol and 10 fmol for Clonidine (exact mass: 229.0 Da) and Angiotensin II (1046.2 Da), respectively. Detailed mechanism for the laser desorption/ionization process is presented.

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On-Line Metal/CNT Nanocomposite Preconcentrator for the GC Analysis of VOCs in Air Samples

오준식, 이명기, *구영미, **박한오, 정광우

*원광대 화학과 *(주)바이오니아 유전자시스템사업부 **(주)바이오니아*

A miniature on-line sorption trap is used to preconcentrate volatile organic compounds (VOCs) from large-volume air samples and inject the organic compounds into the separation column of GC as a relatively narrow vapor plug. Candidate adsorbents, such as CNT-Co, Ni, Co, Al metal nano-composites, were assessed on the basis of thermal-desorption bandwith and enrichment efficiency, chromatographic peak shape, and breakthrough volume against mixture of organic compounds. The determination of a 26-vapor mixture of common indoor air contaminants in

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Synthesis of Various Nanodiamond Hybrid Nanostructures and Their Photocatalytic Activity

장동명, *송윤미, 김윤희, 명윤, 조용재, 김한성, 박정희

*고려대 소재화학과 *고려대 소재화학과 태양에너지소재*

Cadmium sulfide (CdS), lead sulfide (PbS), platinum (Pt), and gold (Au) nanocrystals were grown in situ on acid-purified detonation nanodiamonds (diameter = 5 nm) by the solvothermal method. These nanodiamond hybrid nanostructures exhibit excellent photocatalytic activity toward the degradation of methylene blue under visible or UV-visible light irradiation, which is comparable to the TiO_2 hybrid ones. In addition to their large surface area advantage, the surface carbons can induce an efficient interfacial electron transfer process that is responsible for the enhanced photocatalytic activity.

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Heterogeneous reaction of ozone with $ChlSO_4$/POPG lipid layer: Perspective from molecular dynamics simulations

최선미, 이영민, 김준곤

포항공과대 화학과

Heterogeneous chemistry is ubiquitous in nature and anthropomorphic processes. For identification of the heterogeneous reactions of biological lipid surfactant layers comprising 1-palmitoyl-2-oleoyl-sn-phosphatidylglycerol (POPG) and cholesterol sulfate ($ChlSO_4$), field induced droplet ionization mass spectrometric (FIDI-MS) technique along with theoretical analysis are utilized. Unique products are observed from the heterogeneous reactions of $ChlSO_4$ and ozone at the air-liquid interface. In addition, the medial location of $ChlSO_4$ in the POPG surfactant layer is investigated via competitive heterogeneous oxidation by ozone. For support the experimental results, we have investigated molecular dynamics (MD) simulations. $ChlSO_4$ and POPG lipid monolayer-water systems were simulated with the all-atom CHARMM22 force field. Indeed, MD simulations results correlate well with experimental observations and provide additional insights into the interactions between lipids and water molecules in the interfacial region.

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Duplex marker detection expressed in breast cancer cells using SERS-fluorescence dual modal nanoprobes

이상엽, *전향아, *주재범

*한양대 응용화학과 *한양대 바이오나노공학과*

The application of metal nanoprobes is emerging as one of the most effective optical imaging tools in the biomedical cancer diagnosis. For example, quantum dots are extensively used as effective fluorescent labels for cellular imaging. However, most of currently available fluorescent organic dyes have relatively weak emission intensities and they are also photo-bleached quickly. In order to resolve this problem, more sensitive and stable probes are still needed. In the present work, dual modal nanopronbes, which can be used for both the Surface-enhanced Raman scattering (SERS) and fluorescence detections, have been developed. SERS detection is a powerful analytical technique that allows ultra-sensitive chemical or biochemical analysis in terms of unlimited multiplexing and single molecule sensitivity. Combining advantages of fluorescence and SERS allow these dual modal nanostructures to be used as powerful probes for a novel biomedical imaging. The proposed fluorescence and SERS dual modal probe which has both advantages of the fluorescence and SERS is one of the most powerful tools because it showed the storage stability, the biocompatibility, and the accuracy for the sample detection. This technique also can be applied various fluorescence and SERS signal obtaining system for multi-marker cancer cell imaging.

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Phosphorylation effects on serine and threonine dipeptide structure

김수연, 조민행

고려대 화학과

To study phosphorylation effect on serine and threonine dipeptide, we carried out pH- and temperature-dependent circular dichroism(CD) and 1H NMR with phosphorylated serine and threonine dipeptide (pSD and pTD). In temperature-dependent CD spectra, there is an isodichroic point. This is the strong evidence that there exist two distinguished conformers, polyproline Ⅱ and β-strand. By using SVD(Singular Value Decomposition) method, we obtained that relative population of two conformer increases or decreases with increasing temperature and pH. And also we calculated thermodynamic properties such as enthalpy and entropy via van't Hoff plot. In 1H NMR spectra, we measured 3J(HN,Hα) coupling constants and chemical shifts. Through analysis of coupling constants and chemical shifts from NMR spectra and SVD analysis from CD spectra for varying temperature and pH, we can observe the information on propensity for intramolecular H-bonding and the difference between pSD and pTD.

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SERS-based Immunoassay Using Hollow Gold Nanospheres for Clinical Serums

전향아, *이상엽, **윤수영, ***최수진, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과 **고려대 의학과 ***고려대 진단검사의학과*

A quick and reproducible surface-enhanced Raman scattering (SERS)-based immunoassay technique, using hollow gold nanospheres (HGNs) and magnetic beads, has been developed for a clinical sample analysis. Here, clinical samples from patients were provided by Korea University Hospital. Magnetic beads and hollow gold nanosheres were used as supporting substrates and SERS probes for the formation of the immunocomplex, respectively. This SERS-based immunoassay technique overcomes the problem of slow immunoreaction caused by the diffusion-limited kinetics on a solid substrate because all of the reactions occur in solution. For the validation of our SERS immunoassay, well-known lung cancer markers, alphafeto protein (AFP) and carcinoembryonic antigen (CEA) in clinical serums, obtained from 30 patients, were quantitatively analyzed and compared with the clinical data measured by a conventional ELISA method. The SERS-based immunoassay shows a strong potential applicability for clinical blood test.

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For investigation of unfolded state: polyproline II propensities of Blocked shortpeptides using NMR study

오광임, 조민행

고려대 화학과

detailed: blocked GX, XG systems or Homodipeptide systems.overall propensites of dipeptides.

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SERS-based immunoassay using gold-array embedded gradient chip

이문권, 최남현, 주재범

한양대 바이오나노공학과

This study reports a new immunoassay technique using a gradient microfluidic channel and a surface-enhanced Raman spectroscopy (SERS). In this work, we designed and fabricated a 2-fold logarithmic gradient chip to generate various concentrations of a specific cancer marker. In addition, the Au array coated glass substrate and Au nanoparticles were used for a highly sensitive SERS detection. The Au film was modified by self-assembled monolayer methods using 11-mercaptoundecanoic acids. Then capture antibodies were immobilized on hydrophilic Au arrays by covalent bonding. Hollow gold nanospheres (HGNs), conjugated with specific Raman reporters, have been used for the SERS signal enhancement. We have used this method for the quantitative analysis of a lung cancer marker, AFP (α-feto protein), by forming self-assembled sandwich immunocomplexes on Au arrays embedded in a micro-gradient channel. All the solutions were precisely controlled by micro-syringes and infusion pumps. This conceptually new gradient chip-based immunoassay method is expected to be a powerful clinical tool for reliable and sensitive disease diagnosis.

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Phase Behavior of a Room-Temperature Ionic Liquid Confined between Graphene Bilayers : MD Simulation study

조성식

서울대 화학부

Phase transition of liquids confined in nanopores deserves much interest because of phase transition temperatures and phases that cannot be observed in bulk liquids. In spite of many experimental and simulation studies, there are only a few quantitative analyses of relations between confinement and phase behaviors. Using MD simulation technics, we investigated phase transitions of ionic liquid [emim][BF4] (1-ethyl-3-methylimidazolium tetrafluoroborate) which is confined between two graphene sheets. [emim] cation near graphene sheet forms layer structure easily because of its flat structure and aromaticity. We investigated structure and dynamics of such layers within different confinements. Degree of confinement is decomposed into liquid-wall interaction(force field parameters) and liquid-liquid interaction which is very sensitive to number density of liquid molecules. We studied effects of liquid-wall, liquid-liquid interaction, and their combined effects on phase transition of our model confined liquid.

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In Silico Study of Full-Length Aβ42 Oligomers

이제욱, 함시현

숙명여대 화학과

Ab42 oligomers are considered to play crucial roles in the pathogenesis of amyloid-related neurodegenerative diseases including Alzheimer's disease (AD). Many experimental and theoretical studies have been conducted to determine and analyze the structure of Ab42 aggregates. But it has been little known for the structural dynamics, association and dissociation process, characteristic structural features. In this study, using all-atom MD simulation method, we explored the contributions of the different structural elements of full-length A′ 42 oligomers and mutant oligomers (K28G, up to pentadecamer) in aqueous solution to their stability and conformational dynamics. According to the results from our MD simulation studies, 1) b1 region was much more stable than b2 region, 2) D23-K28 salt-bridge was important to maintain the fibril structure.

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Elucidating the Association and Dissociation Mechanism of β-Amyloid Protein by Targeted Molecular Dynamics Simulations

이제욱, 함시현

숙명여대 화학과

The amyloid-b (Ab) proteins are responsible for amyloid plaques in Alzheimer's disease and have been the most widely studied subject in the process of fibril growth. Although much progress has been made to elucidate amyloid fibril properties at a molecular level, the full identification and characterization of all the conformational states and oligomeric structures in the aggregation process and all the conformational changes that link between those different states are still needed to be revealed. Here, we present the results of targeted molecular dynamics (TMD) simulations with explicit water to investigate the structural and mechanistic aspects of the association and the dissociation of the Ab42 dimer. We will discuss the reversibility and the driving forces of the Ab42 dimerization process with several order parameters along the protein aggregation pathway. Also, solvation free energies of Ab42 dimer depending on each association and dissociation process will be discussed in this study.

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Effects of the Structure and Molecular Interactions on the Electrical Percolation Threshold Concentration of Carbon Nanotube/Polymer Composites : Monte Carlo simulation and Percolation Theoretical Studies

이동춘, 권계민, 성봉준

서강대 화학과

Carbon nanotubes (CNT) have received enormous attention due to their excellent optical and electrical properties as conductive fillers. But there have been stumbling blocks because of the strong agglomeration caused by van der Waals force. In order to disperse the CNTs in polymer composites well, either the surface of CNTs is modified by oxidation reaction or CNTs are cut down to smaller picies via sonication so that the strong intermolecular attraction would be slackened. However, the electrical conductivity of CNT-polymer composites can be reduced after such treatments. In this work, we study how the surface modification and the sonication would affect the formation of the electrical percolation network and the conductivity of CNTs in the polymer composites by carrying out Monte Carlo (MC) simulations and locating the electrical percolation networks of CNTs. As the effect CNT aspect ratio and the CNT stiffness changes after the surface modification and the sonication, the electrical percolation threshold concentration of CNTs is increased significantly. The formation of the electrical percolation network of CNTs shows non-monotonic behavior as the intermolecular attraction between CNTs increases. With a weak intermolecular attraction the percolating network of CNTs is formed more easily. However, when the attractive interaction becomes even stronger beyond the critical point, CNTs start agglomerating, thus hindering the formation of a percolating network and as a result, percolation threshold concentration increased significantly. We also calculate structure factors and dynamics of agglomerated CNTs.

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Terahertz Absorption and Emission from Vertically-Aligned Silicon Nanowire and Silicon-Carbon Core-Shell Nanocable Array

서영석, 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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Dominance of Pyridine-like Structure in Highly-Nitrogen Doped Nanosize Graphitic Layers: Experimental and Theoretical Evidence

조용재, 김한성, 명윤, 김창현, 박정희, *강홍석

*고려대 소재화학과 *전주대 나노신소재공학과*

Nitrogen-doped graphitic multi-layers sheathing the Si nanowires were synthesized by chemical vapor deposition of methane/ammonia mixture, using the pre-grown Si nanowires (synthesized by a metal-nanoparticle-assisted catalytic etching process). The thickness (? 50 nm) and N content (? 15 atomic %) of graphitic layers were finely controlled using the deposition condition. Synchrotron X-ray photoelectron spectroscopy revealed that the pyridine-like N structures are dominant to the graphite-like N structure for the higher doing level of the thinner layers. Raman spectroscopy supports the selective growth of two N structures upon the change of the shell thickness and N content. The first principle calculation of carbon nanotubes (CNTs) and graphene reveals that the pyridine-like N doping structures, which have divacancies around the doped sites, becomes more favorable than the graphite-like one at the higher N doping levels.

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FT-IR measures spectral peak of N-methylacetamide-d7 in water mixed with THF

이가연, 조민행

고려대 화학과

N-methylacetamide(CH3CONHCH3,NMA) is the simplest molecule containing peptide units. In this study, we observed frequency of deuterated NMA(CD3COND(CD3), NMA-d7) and NMA-d6 in water mixed with THF via FT-IR. Amide I assigned to the C=O stretching vibration. Amide II band exhibit NH2 bending. The NH stretching vibration in NMA-d6 and ND stretching vibration in NMA-d7 give rise to the Amide A and Amide A' mode. This paper applied to compare peaks of the amide I band, amide II band, and amide A band of NMA-d7. We analyze amide spectral peaks versus the mole fraction of the NMA-d7 in solution.

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Composition control in chemical vapor transport grown GaAs1-xPx nanowires

공강준, 김한성, 정찬수, 박정희

고려대 소재화학과

대한화학회 THE KOREAN CHEMICAL SOCIETY

Ternary GaAs1-xPx nanowires (NWs) with uniform and controllable compositions (0< X

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Growth of carbon nano tube forests on texturized Si substrate

장미라, 이휘건

한양대 화학과

Carbon nano tube 는 흑연면(graphite sheet)이 나노 크기의 직경으로 둥글게 말려 관 모양을 이루고 있으며 관의 지름이 수～수십 나노미터에 불과하여 carbon nano tube 라고 일컬어지게 되었다. magnetron sputtering 방법으로 Al 층과 Fe 촉매를 증착한 후 LPCVD(low pressure chemical vapor deposition)을 아세틸렌(C2H2)가스를 이용하여 carbon nano tube 를 성장시켰다. CVD 로 carbon nano tube 를 성장 시킬 때 흑연면(graphite sheet)이 말리는 각도와 구조에 따라서 금속 또는 반도체의 특성을 보인다. 하지만 이 흑연면(graphite sheet)의 말리는 각도를 조절 하여 대량 합성하는 것은 아직까지 불가능한 일이다. N-type Si wafer 를 이용하여 KOH-IPA 용액을 이용한 식각(etching)을 통한 texturing 기판을 제작하였다. 용액의 농도와 시간을 달리하여 pyramid size 를 조절하였고 다양한 texturing 구조를 갖는 구조의 기판 형상을 이용하여 실험을 하였다. 다양한 pyramid size 의 texturing 된 기판위에 성장시켰다. 이 성장된 carbon nano tube 가 기판 형상과 그에 따른 Fe 촉매의 결정성에 따라 어떤 특성을 나타내는지 알아보기 위해 전계방출 특성을 실험하였고 분광학 장비(Raman, NIR)을 이용하여 에너지 구조를 비교 분석 하였다.

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Prediction of Liquid Densities using van der Waals surface model

Li Jun, 김창곤, 이해황, *조수경, 김찬경

*인하대 화학과 *국방과학연구소 4기술-2-1*

Prediction of physicochemical properties of high energetic materials (HEMs) is an important task. Especially determination of these properties can help to select promising candidates for further development. We have successfully developed QSPR procedure for solid HEMs and applied to various properties. In this work, we wish to expand this procedure to the liquid HEMs. As a starting point, we collected 303 training set molecules to estimate the liquid densities. All the molecules were optimized at the B3LYP/6-31G(d) level of theory and confirmed as minima by frequency calculations. From the optimized structures, 50 descriptors were extracted and were subject to the multiple linear regressions. The model developed here gave excellent correlations for the training set (r=0.987) and the test set (r=0.991).

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Synthesis and luminescence properties of Eu(II) complex with O-N2O2

정용광, 강준길

충남대 화학과

2-[[[2-[[(2-hydroxyphenyl)imino]methyl]phenyl]imino]methyl]-phenol Schiff-base ligand, O-N2O2, as a tetradentate chelate was synthesized from salicylaldehyde and 1,2-Benzenediamine. The europium complex with O-N2O2 was synthesized through refluxing in basic solution. The synthesized complex was characterization by TGA/DTA, PL, CCD, IR, UV, XPS, 1HNMR and it was found that the 3+ oxidation state of europium was reduced to the 2+ state. The Eu(II) complex excited at UV produced blue emission peaking at λmax = 450~470nm depending on solvent. The blue luminescence of the complex was very bright in THF solvent.

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The role of phenyl substituent on the oxidation of alcohols over oxidized TiO_2(001) surfaces

공자현, *김유권

*아주대 에너지 시스템학부 *아주대 자연과학부*

TiO_2 is widely used in various technologically important areas including heterogeneous catalysis and photocatalysis. Understanding the related reaction mechanism may give a clue to design a better catalyst. In the present study, alcohol adsorption and subsetuent oxidation on rutile TiO_2(001) surface is studied by photoemission spectroscopy (PES) using highly intense and monochromatic soft X-rays obtained from synchrotron radiation. Especially, we compare alcohols with two different substituents, which are benzyl alcohol (C_6H_5-CH_2-OH) and ethanol (CH_3-CH_2-OH). Clean and atomically well-ordered rutile TiO_2(001)-3x1 surface is prepared by repeated Ar^+-sputtering and annealing (900K) cycles. Then, the surface is dosed with O_2 at RT, prior to alcohol adsorption. Our C 1s core level spectra indicate that benzyl alcohol forms oxidized intermediates on the O_2-dosed TiO_2 surface at the substrate temperatures lower than 400 K, while ethanol does not. We attribute the difference between the two alcohols to the electronic effect of phenyl substituent as well as thermodynamic effect.

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Estimation of Heats of Vaporization using QSPR Method

김찬경, 김창곤, 이해황, *조수경, **Li Jun**

*인하대 화학과 *국방과학연구소 4기술-2-1*

Heat of vaporization is one of key factors in developing new high energetic materials (HEMs) and determination of this property can help to select promising candidates for further development. It is well-known that estimation of some physicochemical properties related to the phase change is a difficult task. In this work, we optimized 712 molecules collected from various sources at the B3LYP/6-31G(d) level of theory. These structures were verified as minima from the frequency calculations. As the independent variables, 50 descriptors ranging from 0D to 3D molecular structures were generated. To derive some reasonable QSPR eqs, multiple regressions are tried after limiting the maximum number of independent variables to be 5.

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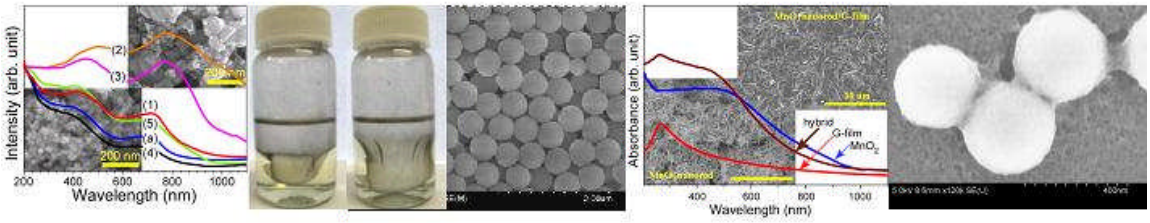
Synthesis and characterization of hybrid silica- and graphene-transition metal oxide materials

도예지, 손영구

영남대 화학과

We have synthesized various silica- and graphene-transition metal oxide hybrid materials and characterized their physical properties by aid of various spectroscopic techniques including scanning electron microscopy, X-ray photoelectron spectroscopy, X-ray diffraction crystallography, Raman, and UV-Vis absorption techniques. Here, we present morphology, interfacial electronic structures, oxidation states, crystal structures, and optical absorption of the hybrid materials.



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Current-Voltage Study from encapsulated β-Carotenes inside single-walled carbon nanotubes

이종택, 이휘건

한양대 화학과

Carotenoids are very important natural pigments in plants and animals and have been used extensively as model systems for the study of π-conjugated polyene molecules. β-carotene is a kind of carotenoids and has many electrons in π-conjugated chains. Therefore if β-carotenes are encapsulated inside single-walled carbon nanotubes, electrons may be transferred between β-carotenes and SWCNTs. β-carotenes were encapsulated in SWCNTs by solution method. And to confirm encapsulation inside SWCNTs, we used UV/Vis, N-IR, and Raman spectroscopy. Then we measured I-V curves after aligning β-carotenes@SWCNTs (β-carotenes encapsulated inside SWCNTs) on Au/Cr electrode. We compared I-V curve on pristine SWCNTs and β-carotenes@SWCNTs and studied electrical property on β-carotenes@SWCNTs

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Laser-induced breakdown spectroscopy of dissolved ions inwater: Signal enhancement and quantification

이용훈

목포대 화학과

Laser-induced breakdown spectroscopy CLIBS) has provided a rapidmulti-elemental analysis tool in the aqueous solution as well as in open air.Therapid identification and quantification of dissolved elements are very useful forenvironmental monitoring , food and drug inspection , and the related industries.However , in the aqueous solution , the LIBS analytical performance is not muc h.satisfactory as in air Clower temperature and short lifetime of plamsa). Inthisarticle , we report LIBS analysis of the Na , K, Ca , and Pb elements in 、y, ate r.Thesub-ppm level detection of alkali metal elements CNa and K) in NaCI and KCIsolutions has been demonstrated. For the heavy metal element , Pb , significantenhancement of the signal-to-noise ratio has been obtained simply by transferringthe sample solution to a filter pape r.Moreover , we suggest a new quantificationmethod of LIBS signals by using the LIBS signal from carbon element as aninternal standard.

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Structures,Energetics and Frequency Analysis of [C6H6]M+ cation isomers(M+=Li+,Na+,K+)

이지현, *서영선, *이기학

*원광대 생명나노화학과 *원광대 화학과*

비공유상호작용은 분자 생물학에서부터 재료디자인 영역까지 현대화학의 많은 영역에서근본적인 역할을 한다.생체분자와 금속 이온의 상호작용에서 π-cation 상호작용이 매우 중요하다. 본 연구에서는 Benzene 과 금속이온(Li+,Na+,K+) 사이의 상호작용으로 부터 형성될수 있는 다양한 이성체의 구조와 진동수 모드를 B3LYP//6-311+G*수준에서 구하였다.이 계산을 통하여 Benzene 의 진동모드에 대한 Li+,Na+,K+의 영향과 cation 의 크기에 따른 이성체들의 상대적 안정도를 분석하였다.

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Electronic structures and Magnetic Properties in $PuSb_xTe_{1-x}$: LDA+DMFT approach

추광호, 심지훈

포항공과대 화학과

We have investigated the electronic structure and the magnetic properties of $PuSb_xTe_{1-x}$ using LDA+DMFT approach. The spectral function of PuTe shows three peaks multiplet structures near the Fermi level and valence fluctuation between f^5 and f^6 configurations. On the other hand, PuSb shows strongly suppressed spectral functions near the Fermi level and much more localized feature with f^5 configuration. We found that the different electronic structures are closely related to the magnetic behaviours of PuTe and PuSb. In PuSb, the ferromagnetic transition is observed with the localized *f* electrons, while the magnetism of PuTe is completely suppressed with the valence fluctuation of 5f electrons. We also discuss the evolution of 5*f* electrons from itinerant to localized behaviour as increasing x in $PuSb_xTe_{1-x}$.

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Synthesis of PbSSe nanowires using vapor transport method and Their Electrical Transport Properties

장소영, 서영석, 박정희

고려대 소재화학과

Ternary alloy PbSSe nanowires were successfully grown through a one-step thermal evaporation route using Au nanoparticles as a catalyst. They consisted of single-crystalline cubic structure nanocrystal (avg. diameter = 200 nm) grown along the [100] direction. The composition was continuously varied from PbS0.6Se0.4, PbS0.2Se0.8, PbS0.25Se0.75, and PbS0.08Se0.92 using the growth condition. The structure and composition were analyzed using X-ray diffraction, high-resolution transmission electron microscopy, electron diffraction, and energy-dispersive X-ray spectroscopy, showing the consistent values of S and Se composition. We fabricated field effect transistors using single PbSSe NWs, which showed intrinsic p-type semiconductor characteristics for all three routes. This finding may be extended for fabricating other composition-tunable 1D ternary alloy nanostructures.

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

Photooxidative Coupling of Thiophenol Derivatives to Disulfides

김형준

단국대 화학과

Disulfide bonds play an important role in determining the structure and stability of proteins and nanoparticles. Despite extensive studies of oxidation of thiols for the synthesis of disulfides, little is known about photooxidation of thiols, which can be a clean, safe, and economical alternative to the use of harmful and expensive metal-containing oxidants and catalysts. In this paper, we report photooxidative coupling of thiophenol derivatives to disulfides. Para-substituted thiophenol derivatives, p-SHC6H4X (X = NO2, COOH, Cl, and OCH3), are irradiated and the disulfides, X2(C6H4)2S2, are identified as major photoproducts using Raman, UV-Vis, IR, and NMR spectroscopy. For p-nitrothiophenol (pNTP), 4,4'-dinitrodiphenyldisulfide (DNDPDS) is produced in 81% yield. The product yield changes with pH, being the highest at pH~5, suggesting that both neutral thiol and anionic thiolate forms of pNTP are required to be present for the photoreaction to occur. Excitation at 455 nm where the thiolate form of pNTP strongly absorbs leads to the largest yield of DNDPDS while very little DNDPDS is formed by excitation of the thiol form of pNTP at 325 nm. Our observations suggest that the photooxidation occurs via collisions of the electronically excited thiolate form of pNTP with the surrounding neutral thiol forms of pNTP. The photooxidation reaction happens regardless of the electron-withdrawing or electron-donating properties of substituents if pH and excitation wavelengths are properly chosen. Versatility of light and generality of the photooxidative coupling reaction of thiophenol derivatives may open new possibilities of selective and site-specific photocontrol of disulfide bond formation in biology and nanomaterial science as well as synthetic chemistry.

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Parametrical Optimization for Generation of High Sensitive SERS Substrate

엄소영, 이유란, 황현석, 김홍래, 권찬호

강원대 화학과

The surface-enhanced Raman scattering (SERS)-active substrates with longlasting stability and easy reproducibility were generated by varying the synthetic parameters of silver sol, which show ~ 4 times higher than the sensitivity of the substrate by the generalized method. The characteristics of the SERS substrate were confirmed through TEM and UV/VIS spectroscopy. SERS spectra of biphenyl derivatives causing the environmental problem are demonstrated by utilizing the high sensitive SERS substrates.

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Synthesis and Characterization of GeBiTe and GeSbTe Nanowires with Memory Switching Effect

정찬수, 박정희

고려대 소재화학과

Solid-state structural transformation coupled with an electronic property change is an important mechanism for nonvolatile information storage technologies, such as phase-change memories. Here we exploit phase-change germanium bismuth telluride (GeBiTe) and germanium antimony telluride (GeSbTe) single-nanowire devices.High-quality nanowires of GeBiTe and GeSbTe, a one-dimensional chalcogenide phase-change nanostructure, were synthesized via thermal evaporation method under vapor-liquid-solid mechanism. The physical morphology, chemical composition, and crystal structure of the as-synthesized GeTe based nanowires were investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy (HR-TEM), and X-ray photoemission spectroscopy.Main device parameters for memory applications such as threshold switching voltage, programming curves, and writing/erasing currents were measured and analyzed. In addition, nanowire-thickness dependent electrical characteristics were measured and efficient lowering of switching power consumption in both GeBiTe and GeSbTe nanowires was observed. Such interesting memory-switching phenomena are compared and discussed in terms of structural, thermodynamic and electrical uniqueness of GeBiTe and GeSbTe materials.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and luminescence properties of Eu(II) complexes with acid organophosphorous

김현준, 장지아, 정용광, 강준길

충남대 화학과

Europium(II) complexes with acid organophosphorous were synthesized and their photophysical properties were investigated. The acid organophosphorous used in this work were Bis(2-ethylhexyl)-phosphate (BEHP) and 2-ethylhexyl hydrogen 2-ethylhexyl phosphonate (EHEP). The synthesized of $Eu(BEHP)_2$ and $Eu(EHEP)_2$ complexes were confirmed with EA, ICP and TGA. The Eu(II) complexes excited at UV produced blue-luminescence, spanning over the 400 – 450 nm region. The quantum yield of $Eu(EHEP)_2$ with Q = 21.2 % is much higher than that of $Eu(BEHP)_2$ with Q = 8.5 %.

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Luminescence properties of 4-hydroxy-5-phenylpyrido[3,2,1-jk]carbazol-6-one : responses to ammonia and water

이효성, 강준길

충남대 화학과

In this study, we synthesized 4-hydroxy-5-phenylpyrido[3,2,1-jk]carbazol-6-one (HPPCO) and investigated its luminescence properties in various organic solvents. HPPCO exhibited very weak luminescence in protic and nonprotic organic solvents. However, the luminescence was markedly enhanced under the existence of small molecules possessing lone-pair electrons, such as ammonia and water. The luminescence sensitivities to ammonia and water in methanol and ethanol were investigated to reveal its capability as a luminescence probe for water and ammonia. Complementing the experimental study, density function theory (DFT) and ZINDO calculations were also performed to determine the configurations of molecular orbitals and transition probabilities for excited states based on optimized structures.

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Synthesis and chracterization of red phosphors for white light emitting diode

유진호, 강준길

충남대 화학과

A red $Ca_{2-x}Ba_xZnS_3:Eu^{2+}$ phosphor was synthesized by the solid-state reaction. The phosphor excited at 460 nm produced the luminescence spanning over the 580 - 730 nm region. The luminescence intensity was enhanced by adding trivalent rare earth ions. 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.

THE KOREAN CHEMICAL SOCIETY

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Photodissociation dynamics of acetic acid at 205nm: The H atom channels

최미현, 신명숙, 권찬호, 황현석, 김홍래

강원대 화학과

Photodissociation dynamics of acetic acid at 205 nm for the $CH_3(C{=}O)O$ + H and $CH_2(C{=}O)OH$ + H channels has been investigated where each channel was identified by deuterium substitution. The H(D) atom spectra were measured by fluorescence at 656.4 nm (Balmer - α line) induced by two photon absorption near 205 nm (1s → 3s, 3d transition). The translational energy releases to the products that were measured by analyses of Doppler profiles in the spectra and the spin correlation arguments suggest that dissociation of acetic acid producing the H atoms should take place on the excited electronic state. The detailed photodissociation dynamics is discussed in relation to the shape of potential energy surfaces.

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2D-IR spectroscopy: scanning polarization-angle

박광희, 조민행

고려대 화학과

2DIR spectroscopy is shown to be experimentally feasible and of use to determine relative angles between a pair of transition dipoles. The transition dipole angles in turn provide structural information on molecules described as coupled anharmonic oscillators. It is shown that either all the diagonal or a selectively chosen cross peak in the measured 2DIR spectra of transition metal compounds can be completely eliminated by properly constrolling the external beam polarization directions. Here, the interesting relationships between beam polarization directions, which are macroscopically controllable variables, and relative angles between a pair of transition dipoles, which are molecular and structural properties in a molecule-fixed frame, are experimentally verified.This novel measurement method combining the polarization angle scanning technique with 2D vibrational or electronic spectroscopy could be a useful tool for probing structural changes of non-equilibrium molecular systems by monitoring the time-dependent changes of angles between transition dipoles.

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Theoretical Study of HOCl, HCl and Cl2 Interacting with Ice Surface

Shoaib Mahbubul alam, *최철호

*경북대 일반대학원 화학과 *경북대 화학과*

We present an ab initio study of the adsorption of HOCl, HCl and Cl2 on ice surface. HOCl, HCl and Cl2 are stratospherically significant compounds and they have been implicated in the stratospheric ozone destruction via a reaction catalyzed on ice surfaces in polar stratospheric clouds. In this study we applied the second –order MØller-Plesset (MP2) level of theory to optimize the geometry using the 6-311++G(d,p) basis set. The binding energies of HOCl, HCl and Cl2 with ice surface were found to be -20.32, -15.78 and -10.94 Kcal/mol respectively. We found higher binding energies from all other previous works that have been done in this field. This is because we have taken a large ice model consists of 484 water molecules to measure the dipole-dipole interaction between the adsorbates and the ice surface. And up to second neighboring water molecules of the adosrbates , we make them fully relaxed to observe the relaxation effect of the ice surface. So the dipole-dipole interaction and relaxation effect have to be considered in order to find the interaction energies of the adsorbates like HOCl, HCl and Cl2 on ice surface.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Headgroup Effect on the Structure of Self-Assembled Monolayers Formed by Cyclohexanethiols and Cyclohexaneselenols on Au(111)

김유영, 강훈구, 이성근, 노재근

한양대 화학과

Surface structures, electrochemical behaviors, binding conditions of cyclohexanethiolate (CH-S) and cyclohexaneselenolate (CH-Se) self-assembled monolayers on Au(111) were investigated by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), thermal desorption spectroscopy (TDS) and cyclic voltammetry (CV) to understand the effect of active headgroup on the formation of SAMs. CH-S SAMs have a closely packed $(\sqrt{11} \times 2\sqrt{6})R30'$ packing structure, whereas CH-Se SAMs have a loosely packed $(\sqrt{30} \times \sqrt{7})R30°$ structure containing unidirectional large ordered domains. We found that CH-S SAMs would prefer to have an upright phase where the molecular backbones are oriented perpendicular to the gold surface, but CH-Se SAMs would prefer to have a striped phase where the molecular backbones are oriented parallel to the gold surface, suggesting that headgroups significantly affect adsorption structure of SAMs.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

DNA Mediated Energy Transfer from Ethidium Bromide to Porphyrins

정진아, 전선희, 김석규

영남대 화학과

Horizontal energy transfer through the DNA stem between simultaneously bound ethidium bromide and porphyrins has been investigated. From earlier study, we reported that the excited energy of DNA bound ethidium bromide 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 long distance DNA bound ethidium bromide mediated energy transfer efficiency. As results, the fluorescence of the DNA bound ethidium bromide was effectively quenched by TMPyP and *cis*-BMPyP. DNA-ethidium bromide, poly[d(A-T)$_2$]-ethidium bromide and poly[d(G-C)$_2$]-ethidium bromide quenching by TMPyP appeared to be upward bending curve in the Stern-Volmer plot. While quenching of the ethidium bromide's fluorescence showed nearly linear curve in the Stern-Volmer plot in the *cis*-BMPyP. The quenching efficiency of DNA bound ethidium bromide complex by TMPyP was significantly decreased, while no remarkable change of quenching efficiency was observed in *cis*-BMPyP case.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

DNA Cleavage by Fenton Reaction;-Effect of Intercalators and Minor Groove Binders

이지훈, *이길준, 김석규

*영남대 화학과 *경운대 한방자원학부*

Reactive oxygen species induce various kinds of damage to DNA, including the modification of the nucleobases and the sugar moiety, resulting in the release of free DNA bases and the cleavage of the single- and double strands. In the presence of transition metal ions, the Fenton reaction is an important pathway for providing the reactive oxygen species. Fenton reaction: $EDTA{\cdot}Fe^{2+} + H_2O_2 \rightarrow EDTA{\cdot}Fe^{3+} + {}^{\bullet}OH + OH^-$In this study, we investigated the effect of the DNA binding drugs to Fenton reaction-driven DNA cleavage reaction. The real time kinetic experiments were performed using linear dichroism (LD). As increasing the concentration of intercalators, ethidium bromide and propidium iodide, the DNA cleavage rate became slow. On the other hand, minor groove binder, 4',6-diamidino-2-phenylindole and spermine, did not affect the cleavage rate.

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Binding mode-dependent fluorescence properties of the meso-Tetrakis(N-methylpyridinium-4-yl) porphyrin- poly[d(A-T)$_2$] complex

GONGLINDAN, 장윤정, 김석규

영남대 화학과

Binding mode of meso-Tetrakis(N-methylpyridinium-4-yl) porphyrin (TMPyP) to poly[d(A-T)$_2$has been known to depend on various factors. One of the factors that dictate the binding mode is the [TMPyP]/[DNA base] ratio (R ratio). At a low binding ratio, TMPyP has been known to bind across the minor groove of poly [d(A-T)$_2$]. Upon increasing the R ratio, TMPyP start to stack along the poly[d(A-T)$_2$] stem. It has been known as the moderate stacking. When the concentration of TMPyP further increases, TMPyP exhibits the tendency to form a TMPyP-DNA assembly, in which TMPyP stacked extensively and the DNA is believed to form a complex along porphyrin assembly. The fluorescence characteristics of the TMPyP including simple emission spectrum, fluorescence decay time, and quenching by NaI and arcylamide were investigated in this work and were compared to those with the TMPyP-d[(A-T)$_6$]$_2$and -d[(A-T)$_3$]$_2$. To the former self-complementary oligonucleotide containing 12 base-pairs, TMPyP has been known to bind in the monomeric manner while to the latter oligonucleotide (6 base pairs), TMPyP purely moderately stacked. This study therefore, allows us to compare the fluorescence properties of TMPyP-poly[d(A-T)$_2$] complex with pure monomeric and moderately stacked TMPyP along the AT base pairs. As the TMPyP-poly[d(A-T)$_2$] complex was excited at 430 nm, it produced emission spectrum in the 600 ~ 800 nm range and was consisted of two strong bands at 657 nm and 716 nm at R ratio of 0.02. The relative intensity of these two peak namely F657nm/F716nm was 1.48. As the R ratio increased, both maxima showed the tendency to shift to the long wavelength and the relative ratio increased to 1.69. Both emission bands become broad with the increasing intensity around 690 nm. The emission recorded from TMPyP-oligonucleotide complex exhibited similar tendency. When TMPyP form a monomeric binding with d[(A-T)$_6$]$_2$, the emission bands were sharper than those stacked. Other fluorescence characteristics will be discussed in the poster section.

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DNA Mediated Energy Transfer from DAPI to Porphyrins and ethidium bromide to Porphyrins

권용준, 정진아, 전선희, 조태섭, 김석규

영남대 화학과

From earlier studies, we studied the effect of 4'6-diamidino-2-phenylindole (DAPI) concentration to the DNA mediated energy transfer efficiency and long distance to the DNA mediated energy transfer efficiency. In that case, we used that the excited energy of DNA bound DAPI and the excited energy of DNA bound ethidium bromide was effectively transferred to porphyrin molecule, that is, meso-tetrakis(N-methylpyridinium-4-yl) porphyrin (TMPyP) or *cis*-*bis*(N-methylpyridinium-4-yl) porphyrin (*cis*-BMPyP). As a result, the fluorescence of the DNA bound DAPI and DNA bound ethidium bromide was effectively quenched by TMPyP and *cis*-BMPyP. DNA-DAPI, poly[d(A-T)$_2$]-DAPI and DNA-ethidium bromide, poly[d(A-T)$_2$]-ethidium bromide, poly[d(G-C)$_2$]-ethidium bromide 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 DNA-DAPI complex and DNA-ethidium bromide complex by TMPyP was significantly decreased, while no exceptional change of quenching efficiency was observed in *cis*-BMPyP case.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Metallic-DNA mediated Energy transfer from Ethidium bromide to Meso-tetrakis (N-methylpyridinium-4-yl) porphyrin

박보라미, *한성욱, 김석규

*영남대 화학과 *경운대 환경공학과*

Contact energy transfer from DNA base to various ligands, which can be represented by the ratio of the fluorescence intensity Q(λ)/Q527nm, is measured by conventional fluorometer. When meso-tetrakis (N-methylpyridinium-4-yl) porphyrin (TMPyP) and ethidium bromide bind to DNA simultaneously, energy is transferred from excited state of ethidium bromide to TMPyP. We found that metallic-DNA (M-DNA), to which divalent metal ions are coordinated, also has a capability to transport an excited energy between simultaneously bound drugs, TMPyP and ethidium bromide. The energy transfer efficiency has been shown to depend on the bound metal type and the mixing ratio, [metal]/[DNA]. Alkaline earth metal ions showed mixing ratio dependent increase of energy transfer efficiency in 0 to 100 μM range. Meanwhile, transition metal ions showed similar increase of energy transfer efficiency but no further increase was observed at higher metal concentration. This difference may be due to the difference of binding mode of both metal ions: alkaline earth metal ions are known to bind at the phosphate group of DNA via electrostatic interaction, while transition metal ions do the DNA bases directly.

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TERS of self-assembled monolayer of aromatic thiols using the tip-surface gap-plasmons

박찬규, 최한규, 박원화, 김지환

고려대 화학과

We demonstrate the efficient tip-enhanced Raman scattering (TERS) spectro-microscopy that is based on the plasmonic interaction between metallic tip (Ag-coated Si-tip) and the Au thin-film (~10 nm). When illuminated by ~1 mW of 632.8 nm radiation, the tip-molecular monolayer-Au thin-film junction produces strong local field and signal enhancement (>> 103) that is sufficient to observe TERS spectra of ~200 numbers of 4-aminobenzenethiols and 4-methylbenzenethiols in less than 1 s of exposure time. To investigate the electromagnetics of the observed TERS signals, the influences of tip-sample distance and the excitation polarization have been measured in detail. The gap-plasmon TERS allows nanometer-scale (~50 nm) chemical mapping of functional groups of densely-packed organic monolayers without significant far-field SERS background.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Single-molecule SERS of Photo-Generated Aminobenzenethiols

최한규, 박찬규, 박원화, 김지환

고려대 화학과

The individual silver nanoparticle (Ag NP) - nitrobenzenethiol (NBT) monolayer - gold thin-film (Au-TF) junctions are illuminated by a laser light (wavelength of 632.8 nm) to induce photo-reduction, and to monitor the surface-enhanced Raman scattering (SERS) from both the reactant (NBT) and the product (aminobenzenethiol, ABT). While the $\nu_s(NO_2)$ peak of the reactant NBTs shows a gradual exponential decay, indicating the pseudo 1st-order decay kinetics of many (~200) molecules at a NP-TF junction, the b2-bands (9b, 3, and 19b) of the ABT product show discrete rise in intensities. This step-wise rise clearly proves that only a fraction (~2% or less) of the ABTs produced has a significant charge-transfer enhancement whereas the rest of the ABT products remain inactive for the charge-transfer.

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Chemical Modification of Azide-Terminated Self-Assembled Monolayers Using Click Chemistry

강훈구, 김유영, 이성근, 노재근

한양대 화학과

The facile approach to fabricating an organic surface terminated by a given functionality is to take advantage of an appropriate molecule with a thiol anchor group. Although surface modification with electroactive monolayers is typically accomplished by synthesizing a molecule with a pendant alkanethiol group, it is difficult to obtain the well ordered self-assembled monolayers (SAMs) simply because it is tethered to a thiol. Recently, Sharpless "click" chemistry, especially the formation of triazoles through the classic Huisgen 1,3-dipolar cycloaddition was attracted much attention because of high-yield coupling reaction, highly specific, and compatible with a wide range of species and solvents. We demonstrate this click reaction by coupling ferrocene and azide-terminated SAMs. After the surface reaction, the modified organic monolayers were analyzed using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and cyclic voltammograms (CV). Under the conditions used in this study, STM, XPS, and CV studies revealed that the ferrocene was successfully grafted by the azide-terminated SAMs.

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Molecular Dynamics Simulation Study of an Anion-Modulated Supramolecular Fluorescence Chemosensor for C60

이지혜, 권찬호, 김홍래, 이창희, 황현석

강원대 화학과

Molecular dynamics simulations are performed to study the sensitivity of an anion-modulated suparmolecular complex. In the complex, a fluoride anion is binding to a calix[4]pyrrole-based fluorescence chemosensor where one of the pyrrole ring is replaced by a pyrene fluorophore. It has been observed in an experiment that the binding of a fluoride anion to the chemosensor increases the affinity of the complex with C60. To verify the binding affinity of the complex with C60, we investigate two systems, one system consisting of only a chemosensor and C60 and the other composed of a fluoride-binding chemosensor and C60. We calculate the binding constant of the complex to C60 for each system.

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Investigation of Polypeptide Fibrillations on Lipid Bilayers Using Fourier Transform Infrared Spectroscopy

허성우, 고재윤, 김성남, 김승빈, 김준곤

포항공과대 화학과

Irreversible protein aggregations and fibrillations are known to cause cellular dysfunctions and neurodegenerative disorders, such as Alzheimers' disease, Parkinson' disease, etc.. We have investigated interactions of α-helical polypeptides with phospholipids and their effects to the conformational changes and fibrillation processes of the peptides using Fourier transform infrared spectroscopy (FT-IR). A homopolypeptide, poly-(L-glutamic) acid (PLGA), is used for the investigation as a model peptide, which is known to form fibrils with an amyloid like morphology. Strong effects of phospholipd head groups to the change of PLGA from α-helix to β-sheet have been observed from FT-IR spectra. For example, the polypeptide undergoes higher conformation changes on 1,2-dipalmitoyl phosphatidylglycerol (DPPG) bilayers than on 1,2-dipalmitoyl phosphatidylcholine (DPPC) bilayers. Further, strong peptide fibrillation is observed on DPPG biliayers. These observations provide additional insights into the interactions between lipids and peptides and the roles of these interactions to the peptide fibrillations.

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Microfluidic approach for quantitative analysis of RNA within a single cell

김동균, *이남기

*포항공과대 I-BIO(시스템생명공학부) *포항공과대 시스템생명공학부/물리학*

We present a method for directly counting RNA molecules obtained from individual cells. A microfluidic device with pneumatically actuated microvalves enables efficient manipulation of single cells and their lysates, thereby minimizing dilution of analytes. Specific RNA molecules can be detected by hybridizing with fluorescently-labeled anti-sense probes. Microchip capillary electrophoresis allows not only the separation of hybridized RNA molecules from fluorescent probes but also the differentiation of multiple RNA species based on their differences in electrophoretic mobilities. It is expected that, using this approach, RNA species of low abundance can be analyzed and the cell-to-cell variation in RNA copy numbers in biological networks can be studied.

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Single-molecule FRET approach for protein structures and interactions

김철희, 류민태, *이병일, **이남기

*포항공과대 물리학과 *국립암센터 연구소 분자종양학연구과 **포항공과대 시스템생명공학부/물리학*

DNA recombination is a fundamental process for the DNA repair in cells. In the case of prokaryote, DNA recombination occurs in two pathways: “RecBCD” and “RecFOR”. Although “RecBCD” pathway has been studied extensively, “RecFOR” pathway is still poorly understood due to its complexity. “RecFOR” pathway consists of RecF, RecO, and RecR proteins, where RecR, forming a ring-shaped tetramer, plays a major role in their functions. The binding mode between RecR and DNA and the location of RecR on DNA are still unknown. In this work, we have prepared fluorescently labeled RecR and investigated the physical interactions of RecR and RecO using single-molecule Alternating-Laser Excitation Fluorescence Resonance Energy Transfer (ALEX-FRET). We found that DR-RecR exists as a dimer in solution, while RecR forms tetramer by RecO. This result shows that ALEX-FRET is a useful tool for investigating the protein structures and interactions.

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Revealing the sequential mechanism of synaptic vesicle fusion from the docking to fusion by single-vesicle assay

김재열, *최봉규, **이남기, ***김선애, ***신연균

*포항공과대 물리학과 *포항공과대 I-BIO/시스템생명공학부 **포항공과대 시스템생명공학부/물리학 ***Iowa State University, USA*

Synaptotagmins are membrane protein that regulates membrane docking and fusion by interacting with SNARE proteins, the key elements in membrane fusion. Because of its specific Ca2+-binding affinity, synaptotagmin has been suggested as a Ca2+-sensor for membrane fusion. Although synaptotagmin has been studied intensively for a decade, the molecular mechanisms of synaptotagmin in fusion are still poorly understood. In this work, we studied the role of synaptotagmin in vesicle docking and fusion. Here, we used reconstituted vesicles and a single-molecule technique, alternating-laser excitation (ALEX). We observed multiple modes of synaptotagmin interactions according to SNARE assembling and Ca2+-triggering. From our findings, we suggested a noble model for synaptotagmin function in membrane docking and fusion.

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A new approach for single-vesicle fusion: ALEX-FRET

최봉규, *김재열, **김선애, **신연균, ***이남기

*포항공과대 I-BIO/시스템생명공학부 *포항공과대 물리학과 **Iowa State University, USA ***포항공과대 시스템생명공학부/물리학*

At the synapses of neuron, neurotransmitters, confined within lipid vesicles, are released by the way of vesicle fusion. Since the lipid vesicle fusion does not occur by itself, neuron uses machinery proteins, named SNAREs, to induce fast vesicle fusions with the arrival of action potential. This process of fusion can be realized in solution by constructing lipid vesicles with purified proteins. Here, we used a single-molecule technique, named alternating-laser excitation (ALEX), to study single-vesicle fusion in a freely diffusing condition. From this study, we found that homotypic fusion occurs between t-SNARE liposomes (T-T), but not between v-SNARE liposomes (V-V) in the case of neuronal SNAREs. We also found that homotypic T-T fusion of the neuronal SNAREs does not occur in the absence of SNAP-25. These results show that ALEX is a powerful tool for single-vesicle fusion study.

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R2PI and UV-UV Double Resonance Spectroscopic Studies of Jet-cooled Acetaminophen-Water Clusters

민아름, 이승준, 김유식, 문철주, 최명룡, *김성근

*경상대 화학과 *서울대 화학부&생물물리 및 화학생물학과*

Jet-cooled neutral acetaminophen-H2O (AAP-W) clusters have been studied using the REMPI and UV-UV hole burning spectroscopy. The mass-selective REMPI and UV-UV hole burning spectra of the binary AAP-W complexes were obtained. Through the UV-UV double resonance experiments, we have investigated conformational information of AAP-W by fixing the pump laser at the origin bands and scanning the probe laser. We have also calculated the optimized structures of AAP-W by density functional theory (DFT) with a 6-311++G** basis set. Further discussion of this system will be presented.

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Matrix Isolation Infrared Spectroscopy of 2-acetylfuran

이슬기, 정현진, 최명룡

경상대 화학과

Matrix isolation infrared spectrroscopy (MIS) has been used to study the molecular confromations of 2-acetylfuran (2-AF). We have coupled a home built supersonic jet system with matrix isolation FT-IR spectrometry to investigate the conformations of 2-AF at low temperature (10K). Together with experiments, we have also conducted the ab initio calculations to get the conformational information for 2-AF and corroborate the experimental results. The conformational picture of 2-AF will be discussed.

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Infrared Apertureless Near-field Scanning optical microscopy (IR-ANSOM)

김덕수, 김지환

고려대 화학과

We have investigated an apertureless near-field scanning optical microscopy (IR-ANSOM) in the 3~4 um . As a light source, a tunable wavelength change continuous wave infrared optical parametric oscillator (cw-IR OPO) with an output power of up to 20mW in the 3~4 um range has been set up. We carried out sensitively material constrast mapping of near-field around gold nanostructures. we show that IR-ANSOM has the capability of measuring withd sub-wavelength resolution(about 50 nm).

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Matrix Isolation Infrared Spectroscopy of 4-hydroxy-2,5-dimethyl-3(2H)-furanone

정현진, 이슬기, 최명룡

경상대 화학과

Matrix isolation infrared spectroscopy (MIS) has been used to study the molecular conformations of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (HMF). We have coupled a home built supersonic jet system with matrix isolation FT-IR spectrometry to investigate the conformations of HMF at low temperature (10K). Together with experiments, we have also conducted the ab initio calculations to get the conformational information for HMF and corroborate the experimental results. The conformational picture of HMF will be discussed.

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Analysis and control of gene expression noise in bacterial cells

안태기, 김철희, *이남기

*포항공과대 물리학과 *포항공과대 시스템생명공학부/물리학*

Although having the exactly same genome, cells have different level of proteins. This causes significant cell-to-cell variations, which is often called "gene expression noise". Cell noise can be classified into intrinsic and extrinsic noise based on their original sources. In general, extrinsic noise cannot be modeled, because of its diverse noise sources. For a long time, it has been expected that the number of RNA polymerase (RNAP) should be one of the major noise sources, especially when its concentration is relatively low. In this work, we used YFP and other two fluorescent proteins to measure the level of RNAP concentration and noise. We found that RNAP concentration has major effect on the extrinsic noise, but not in the intrinsic noise. Total cell noise increased when RNAP concentration drops under a certain concentration (the critical concentration). This result shows that RNAP plays a critical role on determining the cell-to-cell variation.

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Infrared Spectroscopic Studies of HCl-H2O Clusters in Helium Nanodroplets

이승준, 민아름, 김유식, 최명룡

경상대 화학과

Small (HCl)m(H2O)n clusters have been assembled in He droplets and their spectra in the HCl stretch range (2500-3000 cm-1) have been obtained. In a recent He droplet study [Gutberlet, A.; Schwaab, G.; Birer, O.; Masia, M.; Kaczmarek, A.; Forbert, H.; Havenith, M.; Marx, D. Science 2009, 324, 1545.], a band at 2670 cm-1 was assigned to the dissociated H3O+(H2O)3Cl- ion pair. In this work we have revised the assignment of this band to a cyclic hydrogen bonded form of the (HCl)2(H2O)2 cluster based on careful measurements of the pickup pressure dependence as well as the transition moment angles associated with the HCl stretch vibrations. A number of bands due to small mixed clusters have also been observed. As the number of the captured water molecules increases, a broad feature that spans the 2550-2800 cm-1 range appears. The possible origin of this spectral broadening in large (HCl)m(H2O)n clusters is discussed.

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Reductive dechlorination of Polychlorinated Biphenyls(PCBs) using Fe nanoparticles produced by Pulsed Laser Ablation(PLA)

안아름, 최명룡

경상대 화학과

Polychlorinated biphenyls (PCBs) are ubiquitous environmental contaminants due to widespread use and inadequate past disposal practices. Thus reductive dechlorination of PCBs is important because it removes the chlorine substituents that block aerobic metabolism and reduces PCB toxicity. In this study, we have prepared Fe nanoparticles using an Fe plate via liquid phase - pulsed laser ablation (LP-PLA). The nanoparticles were later palladized, making Fe/Pd bimetallic nanoparticles by redox reactions and played as a catalyst for the dechlorination of PCBs.

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Infrared Spectroscopic Studies of Imidazole Trimer and Imidazole Trimer-Water Complexes

홍성민, 이슬기, 안아름, 이승준, 최명룡

경상대 화학과

We present infrared spectra of imidazole trimer (IMT) and imidazole trimer-water (IMTW) complexes formed in 0.4 K superfluid helium nanodroplets. The structure of IMT was identified by the assignment of the free NH stretching band of IMT using pick-up oven temperature dependence and vibrational transition moment angle (VTMA) experiments. Furthermore, specific free OH and asymmetric stretching band assignments of IMTWs were employed by varying the oven temperatures of imidazole and the pick-up pressures of water. Density functional theory (DFT) calculations were also conducted to help the band assignments.

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LIF, REMPI and UV-UV Double Resonance Spectroscopic Studies of p-Acetaminophenol

김유식, 민아름, 이승준, 최명룡, *이상학, **김성근

*경상대 화학과 *서울대 화학부 **서울대 화학부&생물물리 및 화학생물학과*

In this work, we present the resonant enhanced multi-photon ionization (REMPI), UV-UV hole burning and laser induced florescence (LIF) spectra of p-acetaminophenol(AAP), widely used as a pain reliever and fever reducer. We measured the excitation spectra of AAP monomer using one color resonant two photon ionization (R2PI) from 33400 to 34200cm-1. The spectra are congested mostly due to the methyl internal rotation in the $\pi\pi^*$ state. The UV-UV hole burning spectroscopy convince us that it has only one conformer in the free jet experiment. However, the possible cis or trans conformation of hydroxyl group in AAP may be overlap in the experimental spectrum. Spectral assignments of AAP will be presented with further vibrational analysis from ab initio calculations.

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Solvation dynamics in room-temperature ionic liquids (RTILs) : isoconfigurational ensemble approach

김대건, 정연준, *Hyung J. Kim

*서울대 화학부 *Department of Chemistry, Carnegie Mellon University*

We study solvation dynamics in a room temperature ionic liquid, 1-ethyl-3-methylimidazolium hexafluorophosphate (EMI^+PF6^-), with a diatomic solute pair as a probe molecule by performing molecular dynamics simulations on a coarse-grained model. For a diatomic solute pair, two different state of charge distribution are used, a neutral pair (NP) and a ionic pair (IP) with each atom have opposite unit charge *e* and *-e*. We calculate the normalized time-dependent Stokes shift function in a non-equilibrium solvation dynamics simulation, using a concept of isoconfigurational ensemble to explore the effect of structure in solvation dynamics, after Frank-Condon transition from NP to IP and vice versa, especially in case of $\Delta E_{i\to f}$ equals to zero. $\Delta E_{i\to f}$ is defined by difference of total energy of RTIL-solute system, where i and f mean initial and final solute state. We also perform similar simulation in case of red edge condition and blue edge condition to find specific reasons of dynamic heterogeneity of solvation dynamics.

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Surface Nano-Patterning of CuPc Thin Films Using Various Imprinting Molds Coated with PDMS

홍다정, *류일환, 임상규, *문정호, 도영락

*국민대 생명나노화학과 *국민대 화학과*

Highly ordered patterning of organic thin films in a nanometer scale is desirable for their application in organic photovoltaics (OPVs). In this work, poly(dimethylsiloxane) (PDMS) imprint method has been applied to pattern the surface of copper phthalocyanine (CuPc) thin films. This non-destructive technology is advantageous for the nano-patterning of organic thin films which are significantly vulnerable to the radiation or etchants of conventional lithography. Pre-patterned primary molds, anodized aluminum oxide (AAO) and photonic crystal (PC), were coated with PDMS and used to produce secondary molds, trimethylopropane propoxylate triacryate (TPT) and Norland Optical Adhesive 63 (NOA63). The secondary molds were coated with PDMS and used for surface nano-patterning of CuPc thin films. The surface morphologies of various molds and organic thin films were observed by atomic force microscopy (AFM) and scanning electron microscopy (SEM).

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Vertically aligned ZnO−CdSSe Core−Shell Nanowire Arrays synthesized by chemical vapor transport

최진웅, 명윤, 박정희

고려대 소재화학과

Vertically aligned ZnO−CdSSe core−shell nanocable arrays were synthesized with a controlled composition and shell thickness (10−50 nm) by the chemical vapor deposition on the pregrown ZnO nanowire arrays. They consisted of a composition-tuned single-crystalline wurtzite structure CdS1-xSex (x = 0, 0.5, and 1) shell whose [0001] direction was aligned along the [0001] wire axis of the wurtzite ZnO core. The analysis of structural and optical properties shows the formation of Zn containing alloy in the interface region between the ZnO core and shell, which can facilitate the growth of single-crystalline shell layers by reducing both the lattice mismatch and the number of defect sites. Therefore, the photoelectrochemical cell using the ZnO-CdSSe photoelectrode exhibits high photocurrent and hydrogen generation rate. We suggest that the formation of the CdZnSSe intermediate layers contributes to the higher photoelectrochemical cell performance of the ZnO−CdSSe nanocables.

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Energetic study on impurity atoms in the boundary of bcc/fcc iron system

양혁, 이억균, *이영주

*KAIST 화학과 *포항산업과학연구원 부품신소재연구본부*

The electronic and mechanical properties of iron systems have been of interest for many years. It is well known that grain boundary and stacking fault site acts as crucial factor for mechanical stability of metallic structure. Impurity atoms in the boundary can strengthen or embrittle the whole system. Boron has an extremely good record in improving intergranular cohesion in metals while phosphine causes impurity embrittlement. Hydrogen also makes steel system brittle. Bulk iron contains many other elements. Some of them stabilize and strengthen iron system and some of them don't. We employ a first principles method based on the density functional theory (DFT) with the generalized gradient approximation (GGA) to analyze impurity atoms in iron systems with boundary condition. We calculated grain boundary structures in both of bcc and fcc structure. The impurity atoms are located in substitutional site, tetrahedral interstitial site, or octahedral interstitial site. We consider the impurity atom site according to the atom size and the space in iron lattice structure.

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Effectvie Light Absorption of Organic Thin Films Using PDMS Nano-Imprint Method

김진현, *류일환, *공혜진, *박찬량, 임상규

*국민대 생명나노화학과 *국민대 화학과*

Over the past decade, organic semiconductors have been investigated intensively in a wide range of optoelectronic devices. Especially in organic photovoltaics (OPVs), the energy conversion efficiency was reported to reach 5-6 %. In order for further enhancement, however, it is known that the maximization of light absorption and improvement of the morphology at the electron donor-acceptor interface are necessary. In this work, the surface of PEDOT:PSS thin films, widely used for hole transporting layer between indium tin oxide (ITO) electrode and electron donor material, was periodically patterned using nano-imprint method. The templating master molds were fabricated from PDMS-coated photonic crystals. The light absorption of electron donor thin films deposited on nano-patterned PEDOT:PSS layer was optimized by varying the periodicity and depth of the photonic crystals. This nano-patterning of PEDOT:PSS layer may also alternate the interface morphology between subsequently deposited electron donor and acceptor layers and is expected to enhance the device performance.

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Infrared Photodissociation Spectroscopy (IRPD) and DFT Calculationsof Proton-bound Cytosine, Guanine Homo and Hetero DNA Base pairs in the gas-phase

성연미, *박수진, **한상윤, 오한빈

*서강대 화학과 *서강대 바이오융합학과 **한국표준과학연구원 나노바이오융합연구단*

Extensive studies, both experiments and theory, have been performed for neutral DNA base pairs. However, a little experimental effort has been made for proton-bound DNA base pairs, which may have different binding interactions or structures. In this study, we investigated the gas-phase structures of proton-bound DNA base pairs, particularly, cytosine and guanine, using infrared photodissociation spectroscopy (IRPDS) and B3LYP density functional theory (DFT) calculations with the basis sets of 6-3111+G(d,p) and 6-3111+G(2d,p). We measured the degree of photodepletion of guanine (G), cytosine (C) homo- and hetero-dimers as a function of irradiating IR laser wavelength. The probed wavelength region was 2640–3761 cm-1 which corresponds to C-H/N-H/O-H stretching vibrational modes within dimeric complexes. In three IRPDS spectra for GG, CC, and GC dimers, a couple of photodepletion peaks were observed, which presumably correspond to vibrational features of the above DNA base dimers. These vibrational spectral features were compared with the DFT calculation results, which showed a good agreement to each other. In the poster, we will show the structures of the DNA base pairs obtained by the DFT calculations and further show the details of the experiments.

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Sensitized luminescence and energy transfer of Sm(III) and Dy(III) complexes with β-diketone and phen (phen = 1,10-phenanthroline)

장지아, 정용광, 강준길

충남대 화학과

The complexes of $[Ln(\beta\text{-diketone})_4]^-$ and $[Ln(\beta\text{-diketone})_3(phen)]$ (Ln = Sm and Dy) were synthesized and their photophysical properties were investigated. The β-diketones used in this work were acetylacetone, 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione, 4,4,4-Trifluoro-1-(2-naphthyl)-1,3-butanedione and dibenzoylmethane. The synthesized complexes were confirmed with EA, ICP and TGA. The complexes excited at UV produced sensitized red-luminescence and their luminescence efficiencies were dependent on the ligand. The excitation spectra measured by monitoring the emission proved that the energy transfer took place via the β-diketone ligand, no matter whether phen was included or not in the complex. In this presentation, the energy transfer between the β-diketone ligands and the Ln(III) ions will be precisely discussed.

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Metal ion binding analysis in the [metal ion-IAPP]$^{n+}$ complex by Electrospray Ionization Mass Spectrometry

정상미, 김미지, 김호태

금오공과대 응용화학과

Amyloid deposits of IAPP in the pancreas are an important characteristic feature found in patients with Type-2 diabetes. Human IAPP is extremely amyloidogenic, while rat IAPP do not form amyloid in vitro or in vivo. It is known that a metal ion has an influence on aggregation of IAPP. Copper ion in particular inhibits, Al or Zn ion promotes the formation of IAPP amyloid. However, investigations regarding the [metal ion-IAPP]$^{n+}$ complex have not been conducted systematically using ESI-MS. We present the result of the Ion-trap Electrospray Ionization(ESI) mass spectrometry(MS) study regarding the structure and formation process of metal ion-IAPP(human/rat) complex. The fragment patterns of [metal ion-IAPP]$^{n+}$ complex were analyzed in MS/MS and MS/MS/MS spectra. The metal ion binding site in the [metal ion-IAPP]$^{n+}$ complex is proposed as the results of MS/MS and MS/MS/MS analysis.

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Investigation of [Metal ion + dCMP·dGMP] complexes by electrospray ionization Mass Spectrometry

임유진, 김미지, 김호태

금오공과대 응용화학과

The influence of metal ions upon the characteristics of DNA was investigated over the past 50 years. Specially, Cu^{2+} cation is regarded to associate with DNA base sites by the concentration dependence of the cation. Cation-DNA phosphate interactions are predominant. However, the cation-DNA base interaction is not negligible which can modify the hydrogen bonding that stabilizes the DNA double helix structure. In this study, we investigated the complex structures and binding sites of [CuⅡ+dCMP·dGMP] complex in gas-phase by electrospray ionization mass spectrometry (ESI-MS) using 2'-Deoxycytidine 5'-monophosphate (dCMP) and 2'-Deoxyguanosine 5'-monophosphate (dGMP) for complex formation. MS/MS and MS/MS/MS fragmentation patterns of [CuⅡ+dCMP·dGMP] complex was analyzed by collision-induced dissociation (CID) method in an ion-trap LTQ mass spectrometer. Other metal(Ni^{2+}, Ca^{2+}, Mg^{2+}, K^{+}, Na^{+}) complexes were also investigated for the fragmentation pattern analysis.

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Protein conjugation on nanoparticles investigated by UV-Vis and Raman spectroscopic techniques

박진, 정새로미, 주상우

숭실대 화학과

Recently interest in bioconjugations of proteins on surfaces has increased due to their potential applications in many areas including nanomedicine and surface chemistry. To introduce any required functionalities, it should be a significant step to conduct versatile organic reactions from the self-assembled monolayers on metal surfaces. One of the most versatile methods of bioconjugation may be achieved using 1-ethyl-3-[3-dimethylaminopropyl]carbodiimide hydrochloride (EDC) couplings. EDC is employed as a carboxyl and amine-reactive crosslinker for protein conjugation. Hydrogen bonding-induced redispersion of the aggregated nanoparticles upon protein conjugations has provided a simple and colorimetric tool as an optical sensor to monitor an attachment of proteins on nanoaprticles in an aqueous solution. Conjugation of bovine serum albumin and transferrin on nanoparticles are characterized by UV-Vis, infrared, and Raman spectroscopic tools. Their uptakes into mammalian cells are further investigated by hyperspectral imaging and z-depth dependent confocal surface-enhanced Raman scattering combined with dark-field microscopy techniques.

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RNAi delivery into mammalian cells using chitosan-modified gold nanoparticles

정새로미, 박진, 주상우

숭실대 화학과

RNA interference (RNAi) has emerged as one of the most efficacious therapeutic agents for disease treatments by suppressing specific genes. To enhance its cellular uptake with concomitant gene transfection efficiency, cationic polymers are frequently employed for the RNAi complexes. Chitosan is known to be less toxic and biocompatible positively-charged polysaccharide. Gold nanoparticles (Au NPs) have also attracted much interest in biomedical applications due to their simple synthesis, good biocompatibility, and ease of conjugation of biomolecules. In this work chitosan-capped Au NPs were tested as a carrier for intracellular delivery of RNAi. We examined the suppression and gene silencing for voltage-gated K+ channel proteins in A549 cells by PCR methods. Intracellular distributions of chitosan-capped Au NPs/siRNA complexes have been examined by hyperspectral imaging and z-depth dependent confocal surface-enhanced Raman scattering combined with dark-field microscopy techniques. Our results may suggest that chitosan-capped Au NPs are suitable for intracellular delivery of RNAi for potential therapy.

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Densification of Micro-Nano Rice Husk Silica

zhao yanan, 한종수

전남대 화학과

In recent, we focued on the permeation of RHS membrane modified with silane coupling reagents [(RO)nSiR4-n]. According to the experimental results, we are designing a RHS filter to use for the water filtration. In this study, we made a arbitrary shape from RHS micro-nano particles dispersed in suitable solvent. In the experiment, silane compounds or alkali metal hydroxides were used as coupling reagents, and we got dense shaped RHS sample with high speed centrifugal method. The shape of the samples was not changed by a sintering at 1100°C and the sintered sample has high strength as well as high stability. The results suggested that rice husk silica particles can be molded with high gravitational sedimentation.

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The properties of rf sputtered niobium oxide thin films at different plasma gas ratio

황아름, 박주연, 강용철

부경대 화학과

Niobium oxide thin films deposited on the Si(100) substrates by radio-frequency (RF) reactive magnetron sputtering with different plasma gas ratio mixing argon and oxygen. The deposited niobium oxide thin films were investigated by atomic force microscopy (AFM), scanning electron microscopy (SEM), spectroscopic ellipsometry (SE), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The SEM and SE data showed that the thickness of the niobium oxide films and the thickness was decreased with increasing the oxygen gas ratio. The optical properties, refractive index of the niobium oxide thin films were also studied by SE. AFM images showed that the surface roughness of metallic niobium oxide film. The oxidation state of Nb 3d and O 1s was confirmed by XPS result.

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Investigation of Cobalt Oxide Nanofibers Produced by Electrospinning Process

백정하, 강용철

부경대 화학과

Although cobalt oxides which have chemical activity of cobalt metal are hard to synthesize, in the present study, cobalt oxides have been produced as nanofibers by using electrospinning technique. Cobalt oxides have been interesting because of their exceptional chemical properies. For example, cobalt oxides can be used as electrode materials, magnetic materials, and ceramic industry. Cobalt oxide nanofibers which were produced with a mixed solution of polyvinylpyrollidone (PVP) 0.62 g and different concentration of cobalt nitrate Co(NO3)2 named 0.3, 0.6, and 1.2 g by electrospinning. When the viscosity of the electrospinning solution was high, only nano and submicro-sized cobalt oxide fibers were collected. We applied 0.69 kV/cm of electric field between the needle and the electrically grounded drum collector covered with aluminum foil. Cobalt oxide nanofibers were obtained after calcination of PVP/Co(NO3)2 nanofibers composite at 873 and 1173K. The calcined nanofibers were characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS). XPS experiment performed for investigation of the chemical property of the produced cobalt oxide nanofibers.

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Organic-Inorganic Nanohybrid Nonvolatile Memory Using SAOL-ZnO-Cu layer as Charge Trap Layer by Atomic Layer Deposition

한기복, 성명모

한양대 화학과

The Nano-Floating Gate Memory(NFGM) devices with SAOL(Self-Assembled organic layers)-ZnO-Cu thin film embedded in Al2O3 and AlOx-SAOL were fabricated and the electrical characteristics were evaluated. The Al2O3 layer and AlOx-SAOL were deposited by MLD system and SAOL-ZnO-Cu films were deposited by ALD system. The tunneling layer which is consisted of AlOx-SAOL were sequentially deposited at 100℃. The floating gate is consisted of SAOL and ZnO films, which are doped with copper. The floating gate of SAOL-ZnO-Cu films was used for charge trap. The same as tunneling layer, floating gate were sequentially deposited at 100℃ By using ALD process, we could control the proportion of Cu doping in charge trap layer and observe the memory characteristic of Cu doping ratio. Also, we could control and observe the memory property which is followed by tunneling layer thickness. The thickness of ZnO-Cu films was measured by Transmission Electron Microscopy. XPS analysis was performed to determine the composition of the SAOL-ZnO-Cu film deposited by ALD process. A significant threshold voltage shift of fabricated floating gate memory devices was obtained due to the charging effects of SAOL-ZnO-Cu films and the memory windows was about 13V. The feasibility of SAOL-ZnO-Cu films deposited between Al2O3 and AlOx-SAOL for NFGM device application was also showed.

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Study of Molybdenum Oxide Thin Films by X-ray Photoelectron Spectroscopy

빈준형, 박주연, 강용철

부경대 화학과

Molybdenum oxide thin films were deposited on p-type Si(100) wafer by radio frequency magnetron sputtering method with a metallic Mo target (purity=99.995%). The physical and chemical properties of these films were studied with X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) techniques. The obtained molybdenum thin film at the oxygen ratio of 0% was investigated by XRD which was found to be cubic Mo (110) phase. After the oxygen ratio increased to 5% in the sputter gas, the molybdenum oxide thin films were changed to amorphous phase. The thickness of molybdenum oxide thin films was measured by spectroscopic ellipsometer (SE) and scanning electron spectroscopy (SEM) and the thickness was found to be in the range of 1000nm. When the pressure of oxygen gas in the sputter gas increased, the film thickness was drastically decreased to ca 70 nm. The calculated band gap of the film deduced from SE data increased from 3.17 to 3.63 eV by addition of oxygen in the sputter gas. The roughness of the Mo film was examined with atomic force microscopy (AFM) and it was dramatically decreased after introduction of oxygen. XPS results revealed that the ratio of metallic Mo species in the film decreased but the contents of Mo(VI) species increased as the ratio of oxygen increased in the sputter gas and fully oxidized at low content of oxygen in the sputter gas.

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수산화 인회석에 Ru가 도입된 새로운 이종상 촉매의 합성과 특성 연구

김대현, 권기영

경상대 화학과

특별한 화학약품을 사용하지 않고 공기 중 산소를 이용한 다양한 산화반응이 공업적으로나, 학문적으로 많이 연구되어져 왔다. 우리는 수산화 인회석 (hydroxyapatite) 표면에 Ru 가 도입된 이종상 촉매를 합성한 후, 이 촉매와 공기 중 산소를 이용한 알콜 산화반응에 응용하였다. 우리는 단결정 hydroxyapatite(HAP)를 molten salt synthesis 방법으로 합성한 후, 단결정 표면의 Ca 과 Ru 의 Ion exchange 반응을 이용하여 RuHAP 로 합성하였다. 합성된 RuHAP 를 AFM, ICP, XRD, SEM 를 통하여 분석하였으며, 특히 RuHAP 표면의 미세 구조와 촉매 반응성에 관하여 연구하였다.

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Synthesis and Characterization of Ni Oxide Nanofiber

박주연, 황아름, 빈준형, 강용철

부경대 화학과

The Ni oxide nanofibers were synthesized by sol-gel and electrospinning method with different Ni concentration between 2.73 and 8.18%. The obtained Ni oxide nanofibers were calcinated to remove the PVP compound at 600oC and 900oC. The ultra fine Ni oxide nanofibers were investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The SEM images showed that the Ni oxide nanofibers were successfully prepared by electrospinning technique and the diameters of Ni oxide nanofibers can be measured. XRD results indicated that the crystal structure of Ni oxide nanofibers and the peaks of metallic Ni phase were disappeared with increasing the calcination temperature. XP spectra revealed that the intensity of Ni 2p was increased as Ni concentration was increased and at least two oxidation states of Ni were confirmed.

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Theoretical study for the molecular structures and spectroscopic properties of $C_{60}(CH_2)_nOH$ (n=0-2)

이주영, 김승준

한남대 화학과

Fullerene(C_{60})과 fullerene 을 토대로 한 유도체들은 이들만의 독특한 물리적, 화학적 성질 때문에 응용분야가 매우 다양하며, 특히 fullerenol 은 수용성 유도체로써 생물학적 분야에 응용이 용이하다. $C_{60}(CH_2)_nOH$ (n=0-2) 의 구조적, 열적안정성 및 분광학적 성질을 알아봄으로써 생물학적 분야에서의 응용 가능성을 제시하고자 한다.

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Wavepacket Propagation of Photochemistry with π*→σ* Internal Conversion

안희선, 백경구

강릉대 화학과

Wavepacket Propagation 방법을 사용하여, 먼저 Phenol 의 S_0, $^1\pi\pi^*$, $^1\pi\sigma^*$ 전자상태들이 관여하는 수소해리 반응에 대한 기존의 연구 결과들을 재현하여 다시 검토하고, 이를 확장하여 Phenol-D(C6H5OD)의 wavepacket propagation 을 2-차원 공간(OH bond, CCOH dihedral)에서 수행하여 동위원소 치환이 미치는 동력학 효과를 연구하였다. Adiabatic S_0, $^1\pi\pi^*$, $^1\pi\sigma^*$ PES 를 가지고 chebychev imaginary 방법을 사용하여 S0 의 vibrational eigen-states 들을 계산한 후, 그 initial wave packet 을 사용하여 S_1/S_2 states 의 동역학 과정을 약 400fs 까지 연구하였다. 이를 통해 중수소 치환에 대한 conical intersections 에서의 population transfer 과정 및 nuclear wave packet 등의 변화를 연구하였다. 이러한 방법을 확장 적용하여 n→π* 또는 π→π* 전이로 빛을 흡수한 후, π*→σ* Internal Conversion (IC)을 거쳐 해리가 진행되는 몇 가지 다른 시스템들에 대해서도 연구하여, π*→σ* 광-동력학 과정의 일반적인 특성을 연구하였다.

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Quantum Chemical Study of Reaction Mechanisms of 'R-NCS with R-N_3' and 'Syleneoid with Carbonyls'

김혜미, 백경구

강릉대 화학과

양자화학 계산 방법들을 적용하여 두 종류의 화학반응들을 연구하였다. 첫 번째 종류의 반응은 R_1-NCS 와 R_2-N_3 가 반응하는 경우인데, 한편으로는 R_1 이 일반적인 유기 치환체(Alkyl/Aryl)인지 혹은 유기금속 치환체인지(L_3M, M=Ni, Pd, Pt)에 따라서, 또 다른 한편으로 R_2 가 Na 인지 혹은 H 인지에 따라 확연히 다른 생성물이 얻어진다. 두 번째 종류의 반응은 Syleneoid($TsiSiX_2Li$)와 Carbonly(R_1R_2C=O) 사이의 반응인데, 이 경우에는 Carbonyl 이 Aldehyde 인지 혹은 Ketone 인지에 따라 전혀 다른 생성물들이 얻어진다. 본 연구에서는 이들 두 가지 반응의 가능한 중간체 (Intermediate)들과 전이구조(Transition State)들을 여러 가지 양자화학 계산방법들로 연구하였다. 이를 통하여 이 반응들의 반응 메커니즘을 규명하고, 이들 메커니즘에 나타난 공통점과 차이점에 대한 분석과 정리를 시도하였다.

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Simulation studies on the stability of peptide-base self-assembled nanostructures

박성병, 이명수, 신석민

서울대 화학부

Interests in artificial bionanostructures, including peptide-based self-assembled nanostructures, have been very intense. Recently, Myongsoo Lee et. al. synthesized polymers of ′ beta-sheet-forming peptide (WKWEWYWKWEW) with the hydrophilic oligoether dendron (T3). It was found that the most stable structure for the peptide T3 aggregates is a nanoring structure with highly uniform diameter. Other analogous T-shaped peptides with different relative volume fraction of a dendron to a ′ beta-sheet peptide were found to form aggregate structures other than nanoring formation. We performed MD simulations on the self-assembled structures of the peptide T3 and other analogous peptides using all-atom AMBER force field 96 under the implicit solvation condition. For the peptide without the bulky dendron (T1), bilayer structures of anti-paralle ′ beta-sheet are found to be stable. We examined the stability of various sizes of nanoring structures for T3. Nanorings with ca. 40 monomers of T3 are found to be stable. The simulation shows that the diameter for the inner pore is 3.5–4.5 nm, whereas the whole structure has the diameter of about 11 nm and thickness of about 4 nm, which is consistent with the experimental observations. Analysis on the simulation results suggest that important factors determining the self-assembled structures include H-bonding between backbones of monomers, the electrostatic interactions of Lys and Glu, and the alignments of bulky TRPs. Understanding the basic driving force for the formation of such peptide-based nanostructures is expected to be useful in designing noble functional bionanostructures.

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S_1 state Dynamics of BrXCY(X=F, Cl, Br; Y=O, S) by EOM-CCSD Method

이근혜, 백경구

강릉대 화학과

광-흡수에 의하여 이중결합의 전자가 π^*로 들뜬 다음 $\pi^* \rightarrow \sigma^*$로 상태-간 변환 (Internal Conversion)이 진행된 후, 결합이 해리되는 과정은 광-동력학 연구에서 다루는 중심 내용들 중 하나이다. 본 연구에서는 먼저 Br 원자를 포함하는 여섯 분자들(BrFC=O, BrClC=O, Br_2C=O, BrFC=S, BrClC=S, Br_2C=S)의 저-준위(Low-lying) 전자 상태들(S_0, T_1, S_1, S_2)을 EOM-CCSD 방법으로 연구하였다. 그리고, 특히 S_1 전자상태의 가능한 해리 경로에 대한 PES 를 구하였으며, 해리 경로상에서의 에너지 장벽의 크기와 이 때의 전이상태 분자구조 특성을 구하였다. 이를 바탕으로 광-해리 동력학 과정에 대한 체계적인 분석을 시도하였으며, Br 을 포함하지 않은 경우들과 비교하였다. 실험결과가 매우 제한된 이들 분자들의 경우에 본 연구의 결과들이 이들 전자상태의 동력학 과정을 다루는 보다 본격적인 실험 및 이론 연구의 바탕이 될 수 있을 것이다.

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Expression and Structural Characterization of Ion Channel-forming Transmembrane Protein, hAPP-TM

박태준, 임수연, 김지선, 김용애

한국외국어대 화학과

Numerous studies of APP in the literature to date have focused on its processing at the plasma membrane, its membrane-bound oligomeric state, and the calcium-permeable ion channel formation of non-fibrillar Aβ in the cell membrane. Despite these studies, little is known structurally about the transmembrane region of APP beyond a theoretical model. This is due to challenges in the expression, purification, and sample preparation of eukaryotic membrane proteins. To determine the threedimensional structures of the intact transmembrane domain from human APP (hAPP-TM) and to elucidate the structure and formation mechanisms of the hAPP channel, the isotopically labeled protein must be produced and purified in sufficient quantity. Here, we describe a procedure whereby the hAPP-TM peptide, comprising residues 692–723 of hAPP, was successfully expressed and purified sufficiently to perform NMR analysis. To increase expression levels of the target protein, we designed a construct containing two tandem repeats of the target gene. The fusion protein was expressed in the form of inclusion bodies, purified on immobilized nickel affinity chromatography, and chemically cleaved by cyanogen bromide. Final purification of hAPP-TM was achieved by preparative reversed-phase high performance liquid chromatography (HPLC). The final yields of purified hAPP-TM were around 5 mg/1L of M9 minimal media. Structural characterizations of the hAPP-TM in the membrane-like environments were obtained by circular dichroism, solution and solid-state NMR spectroscopy

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Computational study of fibril-like oligomer formation under the explicit water

김현식

세종대 응용화학과

Aggregation of the proteins/peptides into beta-sheet rich fibril, called amyloid fibril, is a subject of intensive research both experimentally and theoretically. Simulation study of the fibril formation requires heavy computational resources due to time scale of the protein./peptide aggregation. We have performed the computational simulation of peptide aggregation into fibril-like oligomer structure under the presence of explicit water molecules.The current simulation provides insight of protein aggregation into fibrils at the atomic level. Also, the role of water molecules in this fibril formation can be investigated with current simulation.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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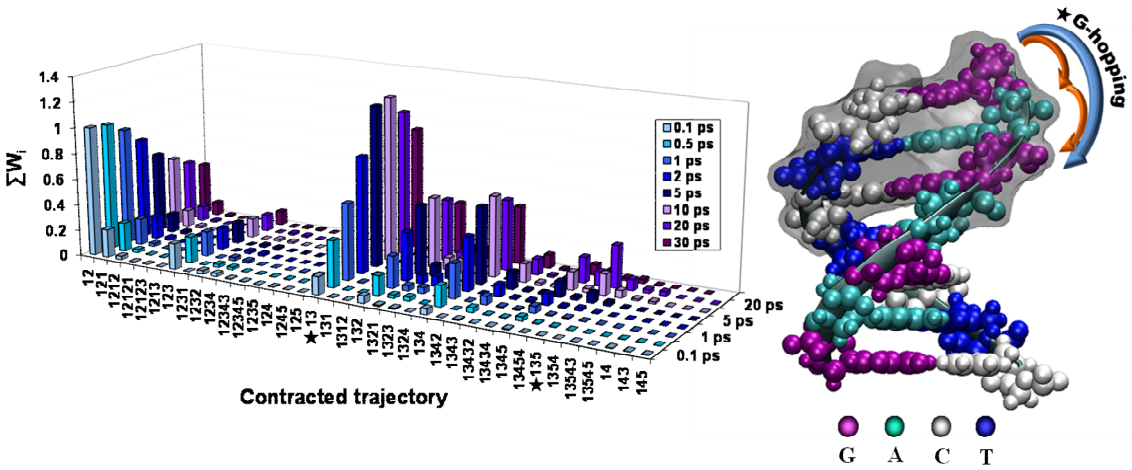
Pathway analysis on long-range DNA charge transfer through adenine and guanine bridges

김희영, 심은지

연세대 화학과

Long-range DNA charge transfer dynamics of 5′-GA_nGA_mG3-3′ (n=1, 2, m=1-3) sequences have been explored on a quantitative basis. First, the degree of coherence was determined in terms of coherence length. Second, relative contribution of charge transfer mechanisms such as incoherent (nearest-neighbor) hopping, through-bridge, and superexchange as well as G-hopping mechanism was assessed by the density matrix decomposition based on the path integral formalism. Finally, time evolution of individual trajectory contribution was investigated through pathway analysis. Although G-hopping pathways were indeed found to be crucial, we have also shown that the initial transfer is driven by the nearest-neighbor hopping pathways through energetically less favored Adenines followed by G-hopping pathways. Therefore, not only the G-hopping pathways but also the through-Adenine pathways govern the overall long-range DNA charge transfer. By placing guanines no farther than two Adenines apart, one can fully utilize efficient tunneling between guanines for long-range DNA charge transfer.



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Spectroscopic Properties of Catechin in Aqueous Solution

박형련, *박철호, **박기민

*전남대 화학과 *남부대 향장미용학과 **경상대 화학교육과*

Catechin is a polyphenolic substance and is also commonly used to refer to the related family of flavonoids and the subgroup flavanols. The substance is contained in a variety of plants such as green tea. It is therefore investigated the spectroscopic properties of catechin in various solvent systems. The substance is soluble in water and it is absorbed below the light of 300 nm. When the substance is dissolved in water, a new absorption peak was appeared near at 350 nm wavelength. Moreover, the absorption spectra of catechin is changed according to the pH values of the aqueous solution. The substance emits weak fluorescence. The fluorescence maximum peaks in water is obtained at 470 nm. Its fluorescence spectra is also changed according to the pH values in the solution.

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Effect of Electronic Coupling Strength on the Degree of Coherence

이지혜, 김희영, 심은지

연세대 화학과

We investigated relationship between electronic coupling strength and the degree of coherence for quantum transport systems. The degree of coherence is quantitatively represented in terms of the coherence length, which is defined as the number of molecular units in which quantum transport process occurs highly efficiently due to strong coherence among them. The reduced density matrix of the transport system is evaluated by means of the recently developed reduced trajectory space analysis combined with the on-the-fly filtered propagator functional path integral formalism. Quantitative estimation of the coherence length is important since it is closely related to charge transfer mechanism and, thus, can give crucial information on designing molecular electronic devices. It was found that coherence length depends significantly on combination of correlation between adjacent couplings in heterogeneous molecular system.

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Investigating Electron Affinity of Molecules: A Density Functional Theory Study

김민철, 심은지, *이동형, *Kieron Burke

*연세대 화학과 *School of Physical Science, University of California, Irvine*

Adiabatic electron affinity of various molecules is evaluated with approximate density functionals. Within the traditional Kohn-Sham density functional theory (DFT), energy of neutral and anion species are calculated with the Perdew-Burke-Ehnzerhof (PBE) exchange-correlation functional and Beck 3 parameterized Lee-Yang-Parr functional (B3LYP). In addition, self-interaction-free DFT energies are assessed by constructing approximate functionals upon Hartree-Fock densities and compared with the traditional DFT results. Comparing the mean average error between calculated electron affinity and experimental electron affinity, it appears electron affinities from Hartree-Fock density derived DFT gives slightly better results than the traditional DFT results for most cases. Tendency of errors are examined and discussed in terms of various criteria (basis set, multiplicity, molecule types and etc.). All calculations were performed with the Jaguar 7.7 program package.

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Fluorescence properties of inclusion complexes of amino- and methoxycoumarins with cucurbit[n]urils

문명구, 강태종

대구대 화학과

Molecular complexation of fluorophores with macrocyclic hosts such as cucurbit[n]uril can affect their fluorescence properties as a consequence of an altered microscopic environment. Cucurbit[n]uril is a relatively new class of host molecules capable of encapsulating guests in a hydrophobic cavity. Cucurbit[n]urils (n=6-8) consists of n glycoluril units bridged by n pairs of methylene groups providing guest binding properties in aqueous media. Compared to cyclodextrin hosts, cucurbit[n]urils are very rigid and have well defined internal cavity. In the present study, we have investigated the complexation behavior of cucurbit[8]uril with practically important fluorescent dyes: 7-aminocoumarins(C120) and 7-methoxycoumarin. These coumarins exhibit fluorescence intensity change in opposite manner upon complexation with cucurbit[8]turil. The fluorescence intensity of 7-aminocoumarin decreases as polarity of medium increases and a large Stokes shift is observed. On the other hand, the fluorescence intensity of 7-methoxycoumarin increases with increasing polarity of medium and the spectral shift is negligible. It is attributed to the modulation of $\pi\pi^*$ state relative to $n\pi^*$ state by the polarity of medium, which is in good agreement with the excited state calculations using DFT method. The fluorescence characteristics of the inclusion complexes indicate coumarins lies in less polar environment than the bulk when complexed with cucurbit[8]uril. The microscopic polarity of cucurbit[8]uril cavity is also under investigation using the pyridinium N-phenolate betaine dye

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Surface-enhanced Raman Scattering of 4,4'-Biphenyldicarboxylic Acid on Ag Island Film

이유란, 엄소영, 황현석, 김홍래, 권찬호

강원대 화학과

The adsorption features of 4-biphenylcarboxylic acid (BPCA) and 4,4'-biphenyldicarboxylic acid (BPDC) on a chemically prepared silver island film were investigated using surface-enhanced Raman scattering (SERS). In SERS spectra of two adsorbates, the lack of the ring C-H stretching vibrational bands and the red shift of the COO^- stretching vibrational bands were observed. To discuss the orientations of BPCA and BPDC on silver island film, the electromagnetic SERS selection rule was adopted with the relative enhancements against the ordinary Raman intensities of the vibrational modes.

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Asymmetry Driven Spontaneous Deformation of Tethered Layer in Dilute Solution

한민우, 심은지

연세대 화학과

Structure deformations of tethered layer driven by asymmetries are studied using dissipative particle dynamics (DPD). We applied both physical and chemical asymmetry on the layer via modifying tether length and tether-solvent interactions, respectively. To prepare well ordered layer structure, we constructed premade layer model with rod-coil molecule which consists of a rigid rod and two flexible tethers. All beads in the layer bonded with harmonic springs to maintain well ordered form. From the model, we found that different deformation process between physical and chemical asymmetry. The physical asymmetry is introduced by reducing the volume of tethers on one side of the layer. It shows spontaneous curved structures and with respect to degree of volumetric asymmetry, various curved structures including hollow tube are obtained. The chemical asymmetry applied by changing tether-solvent repulsion parameter of one side of layer. The modified tethers regarded as hydrophobic chains so they tend to aggregate each other. Consequently, scrolled layer structures with tether filled center are obtained. We found that the physical and chemical asymmetry cause different phenomenon on tethered layer deformation and the results show good agreement with previous experimental data.

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Formation and Kinetics of Self-assembled clusters of AB_2 Miktoarm Star Terpolymers in Various Solvents using dissipative particle dynamics

홍민형

연세대 화학과

Self-assembled clusters of AB_2 miktoarm star terpolymers and their formation mechanism are investigated using Dissipative Particle Dynamics simulations. AB_2 terpolymers are modeled with flexible bead-spring coarse-grained molecules which consist of a hydrophilic A segment and two hydrophobic B segments. In order to explore solvent effects on terpolymer self-assembly, interaction between A segment and solvent-bead is varied with a repulsion parameter: weak repulsion mimics miscible good solvent whereas strong repulsion mimics immiscible bad solvent. It was found that cluster shape alters from spherical micelles at good solvents to vesicles at bad solvents. In addition, To investigate the dynamics of aggregation process with respect to interaction between lyophilic A blocks and solvent C, we evaluated the number of molecules in the lagest cluster of each case. We also investigate comparison between AB_2 miktoarm star terpolymer and linear AB copolymer based on end-to-end distance and morphology. Vesicles are more likely to be formed in miscible good solvent for AB_2 miktoarm star terpolymer.

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Water desalination using CNT membranes

이수인

KAIST EEWS 대학원

Biological pores regulate the cellular traffic of a large variety of solutes, often with high selectivity and fast flow rates. These pores share several common structural features: the inner surface of the pore is frequently lined with hydrophobic residues, and the selectivity filter regions often contain charged functional groups. Hydrophobic, narrow-diameter carbon nanotubes can provide a simplified model of membrane channels by reproducing these critical features in a simpler and more robust platform. Previous studies demonstrated that carbon nanotube pores can support a water flux comparable to natural aquaporin channels. And there are also some researches using CNTs as a ion exclusive membrane. Here, I investigate ion transport through these pores using MD simulations. To mimic the charged groups at the selectivity region, I introduce negatively charged groups at the opening of the carbon nanotubes. To optimize the structure of the CNT, I used QCHEM calculation for each structures which are different each other in the perspective of helicity and spatial structure of negatively charged groups.

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Structural and dynamic properties of a rescaled OSS2 model for water and proton transfer

이송희

경성대 화학과

Classical molecular dynamics (MD) simulations using a rescaled OSS2 model (ROSS2) potential originally derived from ab initio calculations are used to understand the structural and dynamic properties of water and proton transfer in aqueous solutions. The original OSS2 model due to Ojäme et al represents a glassy state. Decreasing the density or increasing the temperature of the system restores normal diffusion, which sug-gests scaling the force field. The O-O, O-H, and H-H radial distribution functions and the self-diffusion coefficients for the ROSS2 potential, obtained by MD simulation, are in good agreement with experiment and calculations for the SPC/E water model. The structure and mobility of the hydrogen and hydroxide ion at infinite dilution using the ROSS2 potential are presented and compared with previous ab initio molecular dynamics (AIMD) studies1,2. The diffusion coefficients of the H+ and OH- ion are in excellent agreement with experiment.

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Synthesis of Sodium Titanate Nanobelts by the Hydrothermal Method

김태완, 강영수

서강대 화학과

The sodium titanate nanobelts were synthesized with hydrothermal process in concentrated aqueous NaOH solution. The products obtained with Ti(O(CH2)3CH3)4 was confirmed to be the crystal structure of Na2Ti2O4(OH)2. The formation mechanism of the crystal structure in the synthetic process depends on various conditions. Their morphology was compared with XRD, TEM, SEM, and TGA. On the basis of their morphology results, nanobelts can be applied for dye sensitized solar cell as electrode by preparing TiO2 nanobelt films on the FTO surface by spin coating and spin coating.Keywords: Sodium Titanate, Nanobelts, Hydrothermal method

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Fabrication of Porous Titania with Controlled Templating Method of Triblock Copolymer for Dye Sensitized Solar Cell

김창우, 문봉진, 강영수

서강대 화학과

We report the mesoporous titania using triblock copolymer as electrode for dye sensitized solar cell. The mesoporous titania was prepared from titanium butoxide using sol-gel process and evaporization induced self-assembly method. The geometrical structure is monitored during the phase-transformation of mesoporous titania synthesized through evaporation-induced self assembly. The phase ordering phase depend on the concentration of polymer and the polystyrene block in the cores of organic-inorganic composite. Mechanisms of formation of the titania meso-structures are proposed and should be very much useful for electrode.Keywords: Mesoporous, Titania, EISA.

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Hematite (Fe2O3) Nanorods with Various Pore Size: Ionic Liquid-Assisted Pore Control

차현길, 강영수

서강대 화학과

The hematite nanorods with various pore sizes have been successfully synthesized via an ionic liquid assisted hydrothermal synthetic method. The samples are characterized by X-ray diffraction, scanning electron microscopy (SEM), transmission electron microscopy and high-resolution transmission electron microscopy. The results indicated that the as-prepared samples are hematite porous nanorods with various pore sizes. The effect of the ionic liquid 1-n-butyl-3-methylimidazolium chloride ([bmim][Cl]) on the formation of the hematite porous nanorods. The proposed mechanism has also been investigated on the basis of a series of TEM studies of the products obtained at different calcination temperature and TGA-DSC results. The UV-vis measurement suggests that the as-synthesized hematite porous nanorods with different pore size possess different optical properties. Keywords: Hematite, Ionic Liquid, Porous materials.

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Synthesis of CuO Grafted TiO2 Nanorod Arrays and Fe2O3 Grown Grafted TiO2 Nanowire Arrays Directly on Transparent Conducting Oxide Coated Glass

강동인, 차현길, 강영수

서강대 화학과

Single-crystal one-dimensional (1D) semiconductor architectures are important in materials-based applications requiring a large surface area, morphological control, and superior charge transport. Titania has widespread utility in applications including photocatalysis, photochromism, photovoltaics, and gas sensors, photoelectrochemical devices, but is activated only by irradiation with ultraviolet (UV) light. Thus, visible light-sensitive TiO2 photocatalysts are required to efficiently utilize solar energy and indoor light, and numerous studies have investigated such photocatalysts. It has been investigated TiO2 nanorods with grafted visible light sensitized metal oxides and these materials were found to be sensitive to visible light. These metal oxide grafted TiO2 nanorods can be used as the photocatalyst or the electrode of DSSC.

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Sonication Induced Synthesis of Purely Red Emitting Y2O3:Eu3+ Nanophosphors

Abhijit Pandurang Jadhav, Amor Uttaam Pawar, 강영수

서강대 화학과

Homogeneously distributed nanoparticles of europium doped yttrium oxide (Y2O3:Eu3+) were synthesized by sonication method. The morphology of as synthesized red phosphor was studied on the basis of variation in pH of the solution and different sonication time. The variation in pH values was responsible for preferential crystal growth in (321) direction. The amount of concentration of incorporated activator ions in the host crystal was responsible for variation in emission intensity of the phosphor as well as decay time. The ultrasound driven growth of nanoparticles and respective crystal structure was studied on the basis of reaction time and synthesis conditions. The emission intensity at 612 nm shows presence of Eu3+ state of activator europium in the host crystal.Keywords:Sonication method, Y2O3:Eu3+, red phosphor, decay time.

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Preparation of Phosphor Nano Composite Polymer Film using CMS Phosphor for Green House Application

Amor Uttaam Pawar, Abhijit Pandurang Jadhav, 강영수

서강대 화학과

Eu doped CaMgSi2O6 nanoparticles were synthesized by co-precipitation method. These nanoparticles were calcined in presence of N2-H2 (96-4%) at 1100 oC for 2 hrs and showed blue emission at 337 nm excitation wavelength. When the calcination was carried out, Eu2+ state of europium is responsible for blue emission phosphor. These synthesized nanoparticles incorporated with EVA and LDPE polymer and prepared film using Carver hot press machine and Blow-extrusion machine. The prepared film was characterized for percentage transparency, mechanical strength and luminescence activity.Keywords: Blue phosphor, CaMgSi2O6:Eu2+/3+, Polymer film.

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Facile Synthesis of Monodispersed Cubic CdS Crystal Cluster: A Free Surfactant Method

Pham Quoc Long, 강영수

서강대 화학과

CdS nanocrystal clusters were synthesized using a free surfactant method. The facile process was done at 80oC with the mixing of cadmium nitrate and thioacetamide. The clusters are highly monodisperse with average size of 230 nm. XRD and TEM image indicate that the CdS crystals are cubic structure and poly crystal. The photoluminescence spectrum of CdS in water shows the green emission at 518 nm while most works report on the red emission as the size of cluster increases.Key words. Cadmium sulfide, water splitting, nanocrystal clusters.

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Preparation of Nanomaterials by Using Electrodeposition Method

Zheng jin you, 강영수

서강대 화학과

We focus on using electrochemical deposition method to get different structure of metal nanomaterials, such as cubic shape, dendritic structure, and so on. So we want to choose the different kind of solution and different substrate and we also changed the potential, current and some other conditions, such as PH and temperature. We used the deposited materials or electrode for catalyst and solar cell. We used the mixture solution contains CuCl2 and NiCl2 with the concentration ratio (Cu2+/Ni2+=0.14M/0.1M) for the electrolyte. Chronoamperometry was applied to obtain the deposits from the mixture solution using the potential at different times in a stationary electrolyte solution without any stirring or gas bubbling. We obtained a good Cu-Ni alloy dendritic structure film on Cu substrate at -1.5 V for 150 s.Keywords: electrodeposition, dendritic structure, CuNi alloy

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The Synthesis of Anatase TiO2 Single Crystals with Dominant {001} Facets for Photocatalytic Applications

Nguyen ky cuong, 차현길, 강영수

서강대 화학과

Owing to wide-ranging industrial applications and fundamental importance, tailored synthesis of well-faceted single crystals of anatase TiO2 with high percentage of reactive facets has attracted much research interest. In this work, single crystalline anatase TiO2 have been prepared by using hydrothermal conditions with precursor TiF4. Fluorine species (herein HF) are introduced as a stabilizing agent to reduce surface energies of anatase TiO2, especially {001} facets, which leads to large percentage of the reactive {001} facets exposed in final titania. Anatse TiO2 single crystals with various degrees of truncation are formed as results of difference in relative concentration ratios between HF and TiF4. The effects of fluorine species and precursor TiF4 against the quality, the size, shape as well as the reactivity of anatase TiO2 crystals have been investigated.

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Preparation and Characterization of One-axis Orientated Array of Cuprous Oxide Nanocrystals

손종화, *강영수

*서강대 화학과 나노구조물연구실 *서강대 화학과*

Cuprous oxide (Cu_2O) nanocrystals were synthesized by precipitation method. Its diameter was less than 500 nm and it has cubic shape. The as-obtained particles were characterized by XRD, SEM, TEM (HR-TEM), SAED, and UV. These products, cubic-shape, show their unique properties as single crystal. The particles were well-orientated by a manual technique upon modified surface of slide glass. The XRD patterns show that one-axis oriented monolayer is dominated by (002) plane. And also we have studied the phase transition of cuprous oxide to form copper oxide by calcination process. As phase is changing, dominated plane is also making changes.

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Structures and Electronic properties of Graphene-Adenine Complex

장성우

경희대 화학과

Graphene, a single atomic layer of graphite, has recently attracted considerable attention due to its remarkable electronic and structural properties. Graphene has the thickness of one atomic scale and remarkable electron mobility. For applying as tumor tracer and finding mismatched DNA, it seems be very important the Graphene-DNA base complexes. In this work, we calculate the interaction between adenine (DNA base) and graphene by using density functional theory (DFT) and with peridic boundary condition (PBC) method, thus we approximate the surface phase of graphene. There are two ways of interaction between graphene and Adenine. First, when the graphene is fully pasivated by H, it interacts with adenine by van der waals force, then the bond length is 3.1 Å and their binding energy is very weak (~0.37 eV). On the other hand, when the two H on the graphene are removed, the bond length is 1.54 Å. It imply that there is a covelent bond. This may derive the strong charge transfer and break the band structure of the graphene.

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가스 하이드레이트 생성 억제제 개발을 위한 연구

김상현, 강완규, 김기섭

충주대 화공생물공학과

친환경 물질로 이온성 액체에 대한 관심이 증가되고 있으며 다양한 분야에서 활용 가능성에 대한 연구가 활발히 진행중이다. 이온성 액체는 비교적 거대 유기물인 양이온과 음이온의 결합으로 이루어져 있으며 다양한 양이온과 음이온의 도입으로 각각에 결합에 따른 다양한 특성을 얻을 수 있다. 본 연구에서는 가스 하이드레이트 생성 억제제로 활용하기 위하여 여러가지의 이온성 액체를 가지고 연구를 진행하였다. 이전에 발표된 dialkylimidazolium 으로 구성된 이온성 액체와 달리 다른 양이온인 물질을 가지고 실험에 대한 결과값을 얻었다. 실험 방법은 이온성 액체를 이용하여 하이드레이트가 생성되는 일정 온도·압력의 상평형 조건을 이동시키는 것과, 하이드레이트가 생성되는 조건에서 일정 시간동안 하이드레이트가 생성되는것을 억제하는 실험을 진행하였다.

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RECOG: A program to recognize molecular structures

윤혁, 김창곤, *조수경, 이해황, 김찬경

*인하대 화학과 *국방과학연구소 4기술-2-1*

We have been working on the development of QSPR methods to predict physicochemical properties of high energetic materials. In this process, it was necessary to deal with a database containing more than few hundred molecules. Our strategy is to optimize all the structures using B3LYP/6-31G(d) method and extract 45 descriptors necessary for the QSPR study. In this work, we developed a program called RECOG, which can derive the descriptors from the Gaussian output files. Especially, the RECOG program can automatically detect total number of rings, PI electrons and rotatable bonds. This program was tested on a database containing ca. 500 molecules and proved to be fast and efficient. This program can be further developed to calculate various properties of molecules based on fragment approaches, such as melting points of molecules.

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S_N2 reactions in ionic liquids: A mechanistic study toward solvent engineering

오영호, *장형빈, **지대윤, *송충의, ***이성렬

*경희대 환경응용화학부 *성균관대 화학과 **서강대 화학과 ***경희대 응용화학과*

In the catalysis of S_N2 fluorination reactions, the ionic liquid anion plays a key role as a Lewis base by binding to the counterion Cs^+ and thereby reducing the retarding Coulombic influence of Cs^+ on the nucleophile F^-. The reaction rates also depend critically on the structures of ionic liquid cation, for example, n-butyl imidazolium gives no S_N2 products, whereas n-butylmethyl imidazolium works well. The origin of the oberved phenomenal synergetic effects by the ionic liquid [mim-tOH][OMs], in which t-butanol is bonded covalently to the cation [mim], is that the t-butanol moiety binds to the leaving group of the substrate, moderating the retarding interactions between the acidic hydrogen and F^-. This work is a significant step toward designing and engineering solvents for promoting specific chemical reactions.

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Investigation of the Imbibition Processes in Cd^{2+}-exchanged Zeolites Y (FAU, Si/Al = 1.56) and Their Crystal Structures

서성만, 임우택

안동대 응용화학과

Three single crystals of excessively Cd^{2+}-exchanged zeolites Y were prepared by the exchange of Na-Y ($|Na_{75}|[Si_{117}Al_{75}O_{384}]$-FAU, Si/Al = 1.56) with aqueous Cd^{2+} concentration of 0.05 M to flow past the crystal for 3 days at 294 and 353 K for crystals 1 and 2 and crystal 3, followed by vacuum dehydration at 1×10^{-6} Torr and 423 K (crystal 1) and 723 K (crystals 2 and 3) for 2 days. They were ion exchanged and vacuum dehydrated to generate $|Cd_{11.5}(CdOH)_{12}(CdOH_2)_{20}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 1, $Cd_{43.5}$-Y), $|Cd_{31.5}(Cd_8O_4)_{1.25}(CdOH)_2)|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 2, $Cd_{43.5}$-Y), and $|Cd_{26.5}(Cd_8O_4)_{2.5}(CdOH)_2)|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 3, $Cd_{48.5}$-Y). Their crystal structures were determined crystallographically using synchrotron X-radiation in the cubic space group *Fd*3-*m*. They were refined to the final error indices R_1/wR_2 = 0.0482/01296, 0.0711/0.1846, and 0.0625/0.1640 using 577, 851, and 849 reflections with $F_o > 4\sigma(F_o)$ for crystals 1, 2, and 3, respectively. The number of Cd^{2+}, H_2O, OH^-, and O^{2-} ions or molecules in the three crystal structures, respectively, are about 43.5, 28, 12, 0; 43.5, 0, 2, 5 and 48.5, 0, 2, 10 per unit cell. In all cases, over-exchange due to uptake of OH^- occurred. In crystal 1, four Cd^{2+} ions per unit cell are at site I, 23 at site I', 0.5 at site II', 5, 4, and 3 at three different sites II, and remaining 4 at site III' positions. Each of twelve OH^- ions coordinates 7 site-I' Cd^{2+} ions and 5 site-II Cd^{2+} ions to give $CdOH^+$ and each 28 water molecules binds to 16 site-I' Cd^{2+} ions and 4 site-III' Cd^{2+} ions. In crystal 2, eight Cd^{2+} ions per unit cell fill at site I, 10.5 and 5 at two distinct sites I', 3 at site II', and 7, 9, and 1 at three different site II positions. In 1.25 of eight sodalite cavities, four Cd^{2+} ions at the second site-I' and four Cd^{2+} ions at the first site-II bind to four non-framework oxide ions to give the larger cationic $[Cd_8O_4]^{8+}$ cluster (symmetry $3m(T_d)$). Remaining two Cd^{2+} ions at the first site-II coordinate two hydroxide ions. Through crystals 1 and 2, zeoltie Y (Si/Al = 1.56) had apparently imbibed six $Cd(OH)_2$ molecules per unit cell; these decomposed upon vacuum dehydration at 723 K to give, with

five additional Cd^{2+} ions, two $CdOH^{+}$, 1.25 $[Cd_8O_4]^{8+}$ clusters. The extent of $[Cd_8O_4]^{8+}$ cluster in zeolite framework, seen in crystals 2 and 3, increases with ion-exchange temperature from 293 K to 353 K; 1.25 to 2.5 $[Cd_8O_4]^{8+}$ clusters per unit cell, respectively.

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Quantum chemical study of the OLED materials tris[4'-(1''-phenylbenzimidazol-2''-yl)phenyl] derivatives of amine and benzene

황태규, *이성렬

*경희대 화학과 *경희대 응용화학과*

Recently, OLED(Organic Light Emitting Diode) has noticed for alternation intensive LCD industry (to fix display and sensors). It has the advantage of cheapness, simple process and compatibility with good mobility materials. In this report, we investigate Alq3{Tris(8-hydroxyquinoline)-aluminum(Ⅲ)}, which is most popular using material by using DFT(TD-DFT) and CIS methods. We reveal that the calculated absorption/emission spectrums are good agreement with experimental result (error ≤ ~10%). For searching the blue color materials, which is the most difficult problem, we also investigate the geometrical structures of ground and excited states, and the absorption/emission spectrums about TPBPA and TPBPB. The calculated absorption/emission wavelengths of TPBPA are 384 and 415 nm, respectively. These are agreement with experimental spectrums (368 and 427 nm). Also about TPBPB, The calculated results, which are 329 (absorption) and 379 nm (emission), are excellent agreement with experimental results (316 and 383 nm).These experiences are expected to contribute the development of the OLED emission materials.

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Crystallographic studies of Li^+-exchanged Zeolites X and Y, $|Li_{92}|[Si_{100}Al_{92}O_{384}]$-FAU and $|Li_{64}Na_6|[Si_{117}Al_{75}O_{384}]$-FAU

김후식, 임우택

안동대 응용화학과

Single crystals of fully dehydrated and fully Li^+-exchanged Zeolite X ($|Li_{92}|[Si_{100}Al_{92}O_{384}]$-FAU) and partially Li^+-exchanged Zeolite Y ($|Li_{64}Na_6|[Si_{117}Al_{75}O_{384}]$-FAU) have been determined by single-crystal X-ray diffraction techniques at 100 K in the cubic space groups Fd3- (a = 24.663(1) Å) and Fd3 -m (a = 24.619(1) Å), respectively. The two Single-crystal structures were refined using all intensities to the final error indices (using only the 1179 and 554 reflections for which $F_o > 4(F_o)$, respectively) R_1/R_2 = 0.0806/0.2596 and 0.0436/0.1602, respectively. In the structure of $|Li_{92}|[Si_{100}Al_{92}O_{384}]$-FAU, 92 Li^+ ions per unit cell are located at three different crystallographic sites. The 32 Li^+ ions at Li(I') per unit cell are located at site I' in the sodalite cavity opposite D6Rs (Li-O = 1.903(5) Å and O-Li-O = 117.9(3)°). The 32 Li^+ions fill sites II opposite double 6-rings in the supercage (Li-O = 1.968(5) Å and O-Li-O = 118.4(3)°). The 28 Li^+ ions at Li(III) per unit cell occupy the 96-fold positions at site III in the supercage (Li-O = 2.09(12) Å and O-Li-O = 98(8)°). In the structure of $|Li_{64}Na_6|[Si_{117}Al_{75}O_{384}]$-FAU, 64 Li^+ and 6 Na^+ions per unit cell are located at two and one different crystallographic sites, respectively. The 32 Li^+ ions fill site I' in the sodalite cavities on 3-fold axes opposite double 6-rings (Li-O = 1.918(4) Åand O-Li-O = 117.8(3)°), 32 Li^+ ions fill site II opposite double 6-ring in the supercage (Li-O = 2.000(4) Å and O-Li-O = 117.4(3)°). The 6 Na^+ ions occupy at site III' (Na-O = 2.55(3) Åand O-Li-O = 79.3(10)°).

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Synthesis and Characterization of Nanocrystalline ZnS: Mn^{2+}

<u>령티빛</u>, 형은수, 김낙중

한양대 화학과

Zinc sulfide doped with Mn is a well-studied material due to its luminescence characteristics among other interesting properties. Therefore, it has potential for its use in several optoelectronic devices such as Alternating Current Thin-Film Electroluminescent. Since the surface energy of the nanoparticles is very high, agglomeration takes place and particle size increases. To avoid this agglomeration, many researchers have used capping agents or surfactants, but it is very difficult to completely washout the capping agents or surfactants. Herein, this work reports on the synthesis nanocrystals of ZnS doped with Mn by chemical method without using any external capping agents. We have also studied the effect of various Mn concentrations on the size and photoluminescence of ZnS: Mn^{2+} nanoparticles. The sample characterization is characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), and Infrared spectroscopy (IR). UV-Visible optical absorption study is used to determine the optical band gap of the nanocrystalline and photoluminescence (PL) spectra of the sample confirm the incorporation of Mn^{2+} in ZnS nanocrystals..

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Synthesis and Characterization of Benzene Sorption Complex of Fully Dehydrated and Fully Mn^{2+}-exchanged Zeolite Y (FAU, Si/Al = 1.56)

Md. Shamsuzzoha, 서성만, *김영훈, 임우택

*안동대 응용화학과 *안동대 환경공학과*

Benzene sorption complex of fully dehydrated and fully Mn^{2+}-exchanged Zeolite Y, $|Mn_{37.5}(C_6H_6)_{24}|[Si_{117}Al_{75}O_{384}]$-FAU, was prepared by ion exchange in a static method of 0.1 M aqueous $Mn(NO_3)_2$ for 20 days, followed by dehydration at 723 K and 1×10^{-6} Torr for 2 days, followed by exposure to zeolitically dried benzene at 297(1) K for 3 days. The structure was determined by single-crystal X-ray diffraction techniques in the space group *Fd*3-*m* at 100(1) K and refined using all intensities to the final error indices (using the 544 reflections for which $F_o > 4\sigma(F_o)$) of $R_1 = 0.050$ (based on F) and $wR_2 = 0.147$ (based on F^2). All 37.5 Mn^{2+} ions are located at four crystallographic sites; 13.5 Mn^{2+} ions are occupied at the centers of the double 6-rings (site I); 4 and 2 Mn^{2+} ions are filled in the sodalite cavity at site I´ and site II´, respectively. The remaining 18 Mn^{2+} ions are in the supercage near single 6-rings at site II. The benzene molecules are found at two distinct sites within the supercages. Eighteen benzene molecules lie on 3-fold axes in the large cavities where they interact facially with the 18 site II Mn^{2+} ions (Mn^{2+}-benzene center = *ca.* 2.53 Å; occupancy = 18 molecules/32 sites). The Mn^{2+} ions at site II extend more *ca.* 0.44 Å inside the supercage from the plane of the three oxygens to which it is bound compared with $Mn_{37.5}$-Y. The remaining six benzene molecules are found in 12-ring planes; occupancy 6 molecules/16 sites where each is stabilized by multiple weak electrostatic and van der Waals interactions with framework oxygens.

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Theoretical investigation of samarium dihalides (SmX_2; X=F, Cl, Br, and I)

김중한, 이윤섭

KAIST 화학과

Samarium dihalides (SmX_2; X=F, Cl, Br, and I) were investigated using the density functional theory (DFT) and high-level ab initio methods. Total seven electronic states of SmX_2 were considered. The ground states of $SmBr_2$ and SmI_2 are $^7B_1$ state. All DFT methods cannot predict the ground states of $SmBr_2$ and SmI_2 correctly. Especially, M06 functional which is recently proposed underestimates the bond angles of SmX_2 compared with those of other DFT functionals and CCSD(T). Only CCSD(T) provides reasonable energy ordering and molecular structures of SmX_2.

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Selective Remove of Metallic SWNT 3D Networks with Hydrogen Plasma

서정은, 여해구, *임아연, **정준모, 이해원

*한양대 화학과 *한양대 에너지공학과 **한양대 화학공학과*

Carbon nanotubes have excellent mechanical and electrical properties, which make them suitable for many potential applications. Generally, metallic and semiconducting single-walled carbon nanotubes(SWNTs) coexist in as-grown materials. However, for applications in nanoelectronic devices it is necessary to fabricate SWNTs that contain only semiconducting SWNTs without metallic SWNTs. Here, we present electrical characteristic of 3-dimensional SWNT networks on Si pillar substrate. And we demonstrate method of selective remove metallic SWNT networks based on a dry etching process of hydrogen plasma. Selective remove of metallic SWNTs 3D networks were characterized using SEM and Raman analysis.

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Chemical Preparation of Ionic Liquid – stabilized Palladium NPs

강완규, 김상현, 김기섭

충주대 화공생물공학과

We have successfully synthesized Ionic Liquid (IL) - stabilized palladium nanoparticles (NPs) by chemical reduction. The particle size was controlled by adjustment of the current density. Transmission electron microscopic (TEM) images showed NPs with average size of 2.4, 3.2, and 3.5 nm were produced depending on the synthetic conditions. The particle size increased with a decrease in the current density and the length of the alkyl chain in the cations. Electron diffraction patterns of the resulting NPs indicated that the particles had a crystalline structure. Overall, the results showed that NPs can be finely tuned according to the kinds of ILs employed and via chemical reduction.

THE KOREAN CHEMICAL SOCIETY

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Ultraviolet photofragment spectroscopy of isolated dibenzo-18-crown-6-ether complexes with alkali metal cations

최대호, 김남준

충북대 화학과

Ultraviolet photofragment spectra of dibenzo-18-crown-6-ether complexes with alkali metal cations (M+-DB18C6, M=K, Rb, and Cs) were obtained in the gas phase using electrospray ionization quadrupole ion-trap reflectron time-of-flight mass spectrometry. The complex ions were produced by electrospray ionization and were stored in the quadrupole ion trap (QIT), which was cooled down to ~10K by a closed cycle helium refrigerator. In contrast to the photodepletion spectra taken at 150 K, the photofragment spectra in this work exhibited well-resolved vibronic peaks. The vibrational progression with an interval of 22cm-1 was also observed and was assigned as the progression of the “butterfly” mode. This mode is found to be strongly coupled to other vibrational modes of the complex ions and the reason for this coupling will be discussed.

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Fabrication of Cobalt Magnetic Nanostructures Using Atomic Force Microscope Lithography

주해나, 윤성훈, 조소희, 정혜수

한양대 화학과

The fabrication of magnetic metal nanostructures has attracted significant interest for possible applications in high-density data storage media, which has patterns of single dot arrays and stores one bit for each particle according to its magnetization direction. In order to fabricate large area high-density magnetic nanopatterns, several methods have been described using interference lithography, X-ray lithography, and nanoimprint lithography. In this study, we demonstrate the fabrication of cobalt magnetic nanostructures using atomic force microscope (AFM) lithography through the electrochemical reduction of cobalt ions coated on a surface. A cobalt ion containing film, a solution of cobalt (II) acetate in DMF was spin-coated on a Si substrate, on which self-assembled monolayers of n-tridecylamine·hydrochloride were added as an intermediate layer to accomplish high spatial resolution in nanoscale. Desired cobalt nanopattern could be produced by tip-induced local reduction, and its physical and magnetic properties were analyzed by SEM, EDX, and MFM images.

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Uncertainty Evaluation in Measurement of Deodorization Efficiency and Dust-cleaning Capacity of Indoor Air Cleaner

황선, *정민석, *김훈식, **최정진

*한국건설생활환경시험연구원 웰빙소재팀 *경희대 화학과 **한국건설생활환경시험연구원 신뢰성평가센터*

최근 화학분석 과정에서의 불확도 산출은 시험 결과의 품질을 평가하는 가장 중요한 방법이 되었다. GUM(Guide to the expression of Uncertainty in measurement)에서 정의한 불확도는 "측정결과에 관련하여 측정량을 합리적으로 추정한 값들의 분산 특성을 나타내는 파라미터라고 정의하고 있다. 불확도를 사용해야 하는 이유는 측정 결과의 품질 관리 및 보증, 국제기구에서 측정 결과의 상호 인정에 필수 요소, 측정 결과의 품질을 나타내는 가장 좋은 수단이기 때문이다. 그러나 화학 분석과정에 불확도 산출 방법을 적용하는데는 통계적이고 공학적인 여러 기법과 전체 관계식의 설정, 불확도 요인의 적합한 선택 그리고 분석 과정의 유효화 인자들의 검증 등 많은 어려움이 존재한다. 실내 공기 중의 오염 물질을 제거하는 장치인 공기청정기의 가장 기본적인 메카니즘은 탈취 필터와 먼지 집진등으로 구성되어 있으며 공기청정기의 성능 평가중 탈취 효율 평가와 입자청정화 시험도 예외는 아니다. 공기청정기 입자청정화 시험에서는 KCl 입자를 분무하여 경과 시간별로 입자 계수기를 통해 입자의 감소 여부를 측정하여 표준사용면적을 산출하게 되고 탈취 효율 평가에서는 대상 가스인 암모니아, 아세트알데히드, 아세트산 세가지 가스를 주입하여 각 가스들의 농도를 분석한다. 분석 방법은 가스검지관 측정법, UV-Vis 측정법, FT-IR 측정법 등이 있으며 측정 기기 별로 다양한 불확도 인자들이 존재한다. 측정시 시료의 채취과정에서 분석과정, Calibration 과정 등 많은 측정 불확도 요인이 있어 이를 잘 파악하지 않을 경우 측정결과의 신뢰성이 크게 떨어질 수 있다. 그러므로 본 연구에서는 공기청정기 성능평가 방법 중 입자청정화시험과 탈취효율 측정에 대해 다양한 불확도 인자들을 살펴보고 이에 따른 최대한의 불확도 요인들을 포함시켜 입자청정화능력값과 탈취효율을 산출하였다.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

A Study on Synthesis of Iron-Hydrotalcite by Electrolysis Method and application for adsorbent

김이영, 최보라, 김태호, 나성옥, 김지혜, 김종원, 정용석, 권수한

충북대 화학과

Hydrotalcite 가 분산되어 있는 용액에 철(Fe)을 전기분해하여 이온을 발생시킨 뒤 Hydrotalcite 표면(층간)에 흡착(치환)시켜 Fe-Hydrotalcite 를 합성해보고, 합성한 Fe-Hydrotalcite 를 흡착제로서의 응용가능여부에 관해 연구하였다. 음이온 포획능력이 뛰어나고 다공성 물질인 Hydrotalcite 는 흡착제로서의 응용가능성이 기대되는 물질로 본 연구에서는 일반 Hydrotalcite 에 전기분해법을 통하여 철을 침착시킴으로써 Fe-Hydrotalcite 를 합성하고, 합성된 Fe-Hydrotalcite 의 흡착능에 대하여 실험하였다. 흡착제로 사용한 Fe-Hydrotalcite 는 전압(10~60V), 반응시간(1~12 시간), Hydrotalcite 의 양(1~5g)을 달리하면서 여러가지 조건에서 Fe-Hydrotalcite 를 합성하여 보고 각각의 조건에서 합성된 Fe-Hydrotalcite 를 흡착제로 사용하여 수용액중의 크롬 6 가 이온을 흡착하여보고 흡착제로서의 Fe-Hydrotalcite 합성의 최적조건을 찾고, Fe-Hydrotalcite 의 흡착 특성과 흡착능에 대해서 연구하여 보았다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Development of simultaneous determination of several synthetic tar color additives in cold syrups by HPLC

황호, *이범규, 이원재

*조선대 약학대학 *조선대 화학과*

A simple and efficient analytical method for the simultaneous determination of seven tar color additives was developed using ion pair high performance liquid chromatography. The conditions for HPLC analysis were as follows: column, μ-Bondapak C18 (10 μm, 300×3.9 mm i.d.); gradient mobile phase, 0.025 mol/L ammonium acetate (containing 0.01 mol/L tetrabutylammonium bromide)-acetonitrile-methanol (65:25:10) as a mobile for fraction A and 0.025 mol/L ammonium acetate (containing 0.01 mol/L tetrabutylammonium bromide)-acetonitrile-methanol (40:50:10) as a mobile for fraction B; flow rate, 1.0 mL/ min; detection wavelength, 254/520/620 nm. We could attain to the detection limits as 0.01~0.05 μg/mL (254 nm) and 0.005~0.01 μg/mL (520 nm) for six red tar color additives, and 0.05 μg/mL (254 nm) and 0.002 μg/mL (620 nm) for Fast green FCF. This analytical method was applicable to determine the tar color additives contained in several commercial cold syrups.

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발표분야: 분석화학
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A study about stability of Ni-hydrotalcite synthesis from electrolytic decomposition process

나성옥, 김이영, 김지혜, 김태호, 최보라, 김종원, 정용석, 권수한

충북대 화학과

본 연구는 니켈금속의 전기분해를 통하여 니켈을 하이드로탈사이트 표면에 침착시킴으로써 하이드로탈사이트와 촉매제를 따로 사용할 필요없이 한 번에 사용 가능한 물질을 만들고, 첨가제로서의 Ni-hydrotalcite 의 안정성에 대해 연구하는데 있다. 실험은 하이드로탈사이트가 담긴 용기안에 니켈판을 담지하고, 일정 온도하에서 일정한 전압을 가해 니켈이온을 발생시켜 Ni-hydrotalcite 를 합성하였다. 또한 실험 시 발생하는 거품을 제거하기 위해 계면활성제를 사용하였다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ANAL.P-5**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

Seasonal monitoring humic acid samples extracted from the Youngsan river and estuary for a year

배은정, 김성환

경북대 화학과

In six sampling sites of the Youngsan river and estuary, humic acid samples were extracted and monitored for a year. The C18 disk extraction method was used for humic acid extraction. The extracted samples were analyzed by negative mode electrospray ionization coupled to high resolution mass spectrometry. As a result, the humic acid samples could be compared at a molecular level. There is little variation observed in the humic acid throughout the year. In addition, the humic acid extracted from the river and estuary had many commonly observed compounds. This study can help to understand the missing connection between riverine and oceanic dissolved organic matter.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Quantitative analysis of turbid suspension and cream samples using Raman spectroscopy

신가영, 정희일

한양대 화학과

We have determined the concentration of active pharmaceutical ingredient (API) in the turbid aceclofenac suspension and urea cream samples using Raman spectroscopy. In the pharmaceutical fields, suspension solution and cream samples are frequently used. For both samples, we have collected Raman spectra using both back-scattering and transmission modes. Although back-scattering mode is usually adopted for Raman spectral collection, it would have a high chance of collecting information only near to sample surface rather than that of whole sample. Alternatively, the use of transmission mode, based on the collection of Raman signal at the opposition side of the laser illumination, could improve the sample representation. The resulting spectra acquired from both collection modes were compared to each other. Finally, using partial least squares (PLS), calibration models were developed using both spectral datasets, and the corresponding results were compared each other.

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Surface Marker of Brain Cancer Stem Cells (CSCs) Detection by Using Surface Enhanced Raman Scattering

김샛별

한양대 화학과

Cancer stem cells (CSCs) are cancer cells that possess characteristics associated with normal stem cells, specifically the ability to give rise to all cell types found in a particular cancer sample. These cells may generate tumors through self-renewal and differentiation into multiple cell types. Such cells are proposed to persist in tumors as a distinct population and cause relapse and metastasis by giving rise to new tumors. Traditional cancer therapies kill rapidly dividing tumor cells but may spare cancer stem cells that can give rise to a new tumor. In theory, killing cancer stem cells should halt a tumor's growth lead to its disappearance. Also, in brain tumor, it was reported that the cell which was revealed brain CSC surface marker, CD133, acts like cancer stem cell and generate tumors. General fluorescence analysis is difficult to detect CSCs because the concentration of CSCs is very low and several separation steps are required. So, surface enhanced Raman scattering (SERS) based detection would be more desirable to improve sensitivity of the measurement. For selective targeting and detection of a brain CSCs using SERS, we have used gold nanoparticle composed of a gold core onto which an optical reporter dye was bonded and targeted to CD133 antigen by antibodies. After the conjugation of the probe, the resulting Raman signal was measured and related analytical performances were evaluated.

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Enzymatically Amplified Detection Method for Protein Biomarkers

심혜림, 이혜진

경북대 화학과

In this poster, we demonstrate a simple enzymatically amplified detection method for the highly sensitive and selective detection of protein biomarkers (e.g., immunoglobuline E, IgE). The detection scheme is based on the formation of sandwich complex through the specific interaction of unlabelled IgE onto the surface immobilized IgE-specific aptamer followed by the specific adsorption of anti-IgE conjugated horse radish peroxidase (HRP). The surface formed “IgE-aptamer/IgE/anti-IgE-HRP” sandwich complex was then reacted with the substrate 3,3’,5,5’-tetramethylbenzidine (TMB) resulting in purple precipitates on surfaces. Both the sandwich complex formation and the surface precipitation were monitored using an optical microscopy as well as a surface plasmon resonance biosensor. In addition, the robust attachment of biomolecules such as antibodies and aptamers on both glass and gold surfaces using prolinker A and B was characterized using quartz crystal balance and atomic force microscopy.

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발표분야: 분석화학
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Analysis of small pyrolysis products of fluoropolymer

김윤기, 최성신

세종대 화학과

A fluoropolymer is a polymer that contains atoms of fluorine. Good thermal stability is a feature of fluoropolymers and in many respects determines their applications. It is known that the thermal stability of polymers of this type is related to the number of fluorine atoms in the repeating unit. Fluoropolymers characterized by superior physico-chemical properties can meet a variety of severe requirements presented by modern engineering. Hence, they have become important artificial materials in science and industry. Pyrolysis-GC/MS has rapidly grown into a powerful tool for the identification of fluoropolymers. Pyrolysis-GC/MS, being able to provide the important composition and structural information of complex rubber and plastic materials, has become a popular technique for the analysis of rubber materials. In this work, We analyzed small pyrolysis products of fluorocopolymer such as poly(vinylidene fluoride-co-hexafluoropropylene), poly(tetrafluoroethylene-co-tetrafluoroethylene perfluoropropyl ether), and poly(ethylene-co-tetrafluoroethylene) using Pyrolysis-GC/MS. And we investigated the influence of pyrolysis temperature on the relative abundances of the pyrolyzates.

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Application of UV absorbers as matrix for MALDI-MS analysis of polybutadiene

정혜승, 최성신

세종대 화학과

For analysis of matrix-assisted laser desorption/ionization-mass spectrometry (MALDI-MS), sample preparation is very important. Matrix, analyte, and cationizing agent solutions should be mixed with proper ratios for efficient ionization. Matrix absorbs UV radiation and then delivers energy to analyte and cationizing agent help cationization of analyte. For using N2 laser (337 nm) as the light source, matrices have to absorb ultraviolet (UV) of 337 nm. In general, ultraviolet light absorber (UVA) is used in polymeric materials for preventing them from degradation by UV radiation in sunlight. Because UVA absorbs UV radiation of 337nm, it is going to role as matrix in MALDI. In this study, we applied UV absorbers as matrix for analysis of polybutadiene (PB). And we examined optimal conditions of PB analysis with silver trifluoroacetate (AgTFA). The UVAs were found to be good matrices for PB analysis using MALDI-MS.

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Comparison of explosives detection in IMS and APCI-MS

김옥배, 김윤기, *최성신, **신명원, **최규섭, **맹석진, **안승건

*세종대 응용화학과 *세종대 화학과 **(주)우주씨앤티 기술연구소*

Trace analysis of explosives is of major importance in two different fields. One is the threat of an illegal use of these compounds, which has led to major efforts in developing explosives detection systems. The other is growing concern about the health risks associated with the release of explosives from military sites and former ammunition plants into the environment. Many methods have been reported for the detection of explosives and various techniques have been comprehensively reviewed in the literature. X-ray screening, fluorescence quenching, neutron and gamma-ray spectroscopy, LC–MS, UV gated Raman spectroscopy, laser induced breakdown spectroscopy (LIBS), electrochemical and immunosensors, chemiluminescence, SPME-HPLC, and GC-ECD are methods proposed for explosive detection. Most of all, ion mobility spectrometry (IMS) has proved to be one of the best methods for the detection of trace level of explosives due to its low detection limit, fast response, simplicity, and portability. And mass spectrometry is an important tool for the detection of analytes and determination of molecular weight of analytes. In this study, we determined the detection limit and reproducibility of IMS and its results were compared with the results of atmospheric pressure chemical ionization mass spectrometry (APCI-MS).

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Analysis of whey proteins (WP) using flow field-flow fractionation (FlFFF) and size-exclusion chromatography (SEC)

강다영

한남대 화학화

Whey proteins (WP) are classified as milk protein and are soluble at pH 4.6 and 20℃. WP's represents approximately 20% of the original milk proteins. Major components of WP include β-lactoglobulin(β-Lg), α-lactalbumin(α-Lac), bovine serum albuin(BSA) and immunoglobulins (Ig). Whey proteins (WP) are of high nutritional values, and have become an important source of functional ingredients in many formulated foods such as ingredients in health-promoting foods. Whey proteins have a tendency to form a gel or aggregates after heat-induced denaturation. The mechanism involved in denaturation of the whey proteins have been extensively studied. And the aggregates and intermediates produced as a consequence of various heat treatments have been well characterized. The influences of pH and ionic environment on heat-induced denaturation and aggregation have also been studied.Processes such as ultrafiltration, ion-exchange adsorption technologies have been employed for the manufacture of whey proteins. During these processes, denaturation of whey proteins may occur. Thus accurate analysis of the whey proteins is required for the optimization of the processes. For accurate analysis of whey proteins, separation of the whey proteins is needed. A number of liquid chromatographic methods including reversed-phase HPLC and Ion exchange techniques have been employed for separation of the whey proteins. In this study, WP's were isolated from raw milk. The isolated WP's and the powder form of WP isolates (WPI) were analyzed using two different separation techniques, SEC and asymmetrical FlFFF(AsFlFFF). The capabilities of the two separation techniques were compared for analysis of whey proteins.

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Separation and characterization of Staphylococcus aureus using gravitational field-flow fractionation (GrFFF)

김지현

한남대 화학과

Staphylococcus aureus is a pathogenic, gram-positive species. In terms of morphology it can be described as a sample of small, sphere-shaped particles approximately 1 in diameter which travel in pairs, long chains, or grape-like bunchesGravitational field-flow fractionation (GrFFF) employs the Earth's gravitational field applied perpendicularly to a thin, empty channel. GrFFF is a simple and inexpensive technique that has shown suitable for the separation and characterization of various micrometer-size particles of various origins. GrFFF has been applied to living samples as cells or parasites because of its simplicity, reduced risk of sample degradation. In this study, staphylococcus aureus cells were cultured, and then analyzed by GrFFF to determine the size distribution. Then the slices of the GrFFF fractograms were taken, and analyzed by optical microscope (OM) to examine the size and the shape of the cells in each slice. The results from GrFFF and OM showed the size and the shape of the cells change with the culturing time, and form aggregates.

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Characterization of fluorescent material-coated pigment particles using flow field-flow fractionation (FlFFF)

안세영

한남대 화학과

Applicability of pigment particles depends on the particles size and the size distribution as the apparent color of the pigment changes with the particle size distribution. The size or the size distribution of the pigment particles are thus important factors in controlling of the color appearance of the pigment particles.Asymmetrical flow field-flow fractionation (AsFlFFF) provides separation of nanoparticles based on their diffusion coefficients (and thus on their hydrodynamic sizes). AsFlFFF has been shown applicable for separation and characterization of various types of water-soluble or organic polymers and colloidal particles. In this study, AsFlFFF was utilized for size-based separation of the fluorescent material-coated pigment particles and for the determination of their size distributions. The results from AsFlFFF were compared with those obtained from dynamic light scattering (DLS) and electron microscopy. For AsFlFFF analysis, an online fluorescence detector was used for sensitive and selective detection of the fluorescent material-coated pigment particles. The advantages and disadvantages of various sizing techniques were compared for determination of the size distribution of the pigment particles.

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Tandem gravitational split Fractionation (GSF)

권민혁

한남대 화학과

In the full-feed depletion (FFD) mode of SPLITT Fractionation (SF), the separation efficiency (or resolution) of the fraction-a (fraction being collected from the top outlet of the SF channel) is inherently higher than that of the fraction-b (fraction being collected from the bottom outlet of the SF channel). In this study, two gravitational SF (GSF) channels were connected online to improve the resolution of SF. In this way, three fractions can be collected instead of two. In this study, two different approaches were taken, where either the fraction-a or the fraction-b from the first GSF channel (GSF-1) was fed into the second GSF channel (GSF-2). When the fraction-a from the GSF-1 was fed into the GSF-2, fraction-1b, 2a, and 2b were obtained, while, when the fraction-b from the GSF-1 was fed into the GSF-2, fraction-1a, 2a, and 2b were obtained. When the fraction-1b of GSF-1 was re-fed into the GSF-2, the separation efficiency of the fraction-2b was increased by 10-15% compared to that of the fraction-1b. The fraction-1a showed the separation efficiency of higher than 95%, while the fraction-2a showed the separation efficiency of about 90%. When the fraction-1a of GSF-1 was re-fed into the GSF-2, the separation efficiency of the fraction-2a was about 5% higher than that of the fraction-1a. The fraction-1b showed separation efficiency of 50% while the fraction-2b showed the separation efficiency of 53%.

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Study on swelling of starch granules using gravitational field-flow fractionation (GrFFF) and Optical microscopy (OM)

서소연

한남대 화학과

Swelling of starch granules accompanying water sorption causes progressive or sometimes abrupt changes in sorption behavior as a result of structural alterations and the possible exposure of new sites with high affinity for water. It is thus of interest to examine the change in size or shape of the starch granules with time.Gravitational field-flow fractionation (GrFFF) utilizes the Earth's gravity as the external field. GrFFF is useful for separation of micron-sized particles with larger particles eluting earlier than smaller ones. Merits of GrFFF include its technical simplicity, low cost to set up, easy to operate and to maintain, and its gentle separation condition that allows analysis of samples such as living cells. In this study, GrFFF was used to determine and examine the change in the size (swelling effect) of the starch granules, Must potato starch and sweet potato starch. Results from GrFFF were compared with those obtained from optical microscope (OM). The starch granules were sampled for 11-12 days. For both starch granules, the mean sizes were increased with the time stored in water.

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Analysis of carboxymethyl starches using flow field-flow fractionation/multi angle light scattering

김선태

한남대 화학과

A corn starch was derivatized with sodium chloroacetate in alcoholic medium under alkaline condition to produce carboxymethyl starches (CMS). Changes in the thermal characteristics and granule structure of the native corn starch and CMS were studied using Thermogravimetric analysis (TGA) and Scanning Electron Microscope (SEM). Asymmetrical flow field-flow fractionation (AsFlFFF) was connected online with multi angle light scattering (MALS) to study the changes in the molecular weight (MW), molecular weight distribution (MWD), and the size distribution of the corn starch during carboxymethylation. The carrier liquid for AsFlFFF was water containing 0.02% NaN3. The ionic strength of the carrier liquid was varied by adding various amounts of 50 mM NaNO3 to find an optimum carrier composition, at which the interactions among the starch molecules and between the starch molecules and the AsFlFFF membrane are minimized. With the field-programming, where the field strength (cross flow) was gradually decreased according to a power function during a run, AsFlFFF allowed determination of MWD of the starches completed within 25 min. It was found that carboxymethylation of starch results in reduction in MW due to molecular degradation by the alkaline treatment. The weight-average MW was reduced to about 4.4×105 from about 7.2×106 when the degree of substitution (DS) was 0.14. It seems AsFlFFF coupled with MALS (AsFlFFF/MALS) can provide a powerful tool for monitoring of the changes taking place in MW and the size of the starch and related materials during derivatization.

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A Ion-Selective Optical Sensor based on fluorescence enhancement of 15-Crown-5-Anthracene for determination of cesium ion

서효숙, *ALAM MD AL MAHMNUR, *이상학

*경북대 센서및디스플레이공학과 *경북대 화학과*

An optical sensor based on a plasticized polymer membrane containing cesium ion-selective fluoroionophore and lipophilic anions for the determination of cesium ions has been developed. In this work, 15-crown-5 derivative including anthracene was used as a fluoroionophore. Emission intensity of the optode membrane incorporating 15-crown-5 anthracene was measured at 500 nm with excitation at 360 nm in the presence of tris-HCl buffer solution. Under optimum experimental condition, the relative intensity was linear with the concentration of cesium ion in the range of 1.0×10^{-4} M to 1.0×10^{-1} M and the detection limit was obtained 4.2×10^{-5} M, as defined by LOD = $3\times S_b/m$ (where S_b = standard deviation of blank signal and, m = slope of the calibration curve). The effects of pH of sample solution on the fluorescent response, the selectivity, response time and reproducibility of the optode membrane were also discussed. The fluorescent optode system shows a high selectivity and sensitivity for cesium ion with respect to other cations such as K^+, Na^+ and Li^+.

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Characterization of LBL Assembly of Metallic Nanomaterials and Biosensing Applications

권민정, 김성엽, 이혜진

경북대 화학과

In this presentation, we demonstrate a simple layer by layer (LbL) assembly method to create biofunctionalized Au and Ag nanostructures on surfaces. Multilayers of Au nanocages or Ag nanocubes were first formed via the sequential adsorption of alternating layers of 1,6 hexane dithiol and Au nanocages or Ag nanocubes on a chemically modified gold surface. The nanostructured mutilayers were then characterized using three different measurements including atomic force microscope, quartz crystal microbalance and scanning electron microscopy. In addition, the multilayers were functionalized with bioreceptors such as antibodies and aptamers which can interact with target proteins and their sensing capabilities were investigated using in-situ surface plasmon resonance as well as various electrochemical methods.

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Synthesis and chromatographic enantiomer separation of γ-lysine functionalized peptide nucleic acid analogs

황호, *조군호, 이원재

*조선대 약학대학 *(주)파나진 -*

Peptide nucleic acids (PNAs) are DNA analogues in which the nucleic acid backbone is replaced by a pseudopeptide backbone and nucleobases are attached to the backbone by methylene carbonyl linkers. γ-Carbon modification of the PNA structure allows monomers, and subsequently oligomers, with improved properties to be obtained. In this study, we report the convenient synthesis of γ-lysine-modified PNA monomers for pyrimidine bases (thymine and cytosine) with high optical purity (> 99.5%) and direct enantiomer separation of γ-lysine-modified PNA analogs, using chiral HPLC to determine the optical purity.

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Matrix-Free Laser Desorption/Ionization Mass Spectrometry on Nanoporous Gold with Different Characteristic Surfaces

진장미, *서보라, *김종원, 김성환

*경북대 화학과 *충북대 화학과*

In this research, nanoporous gold(NPG) surfaces are used for matrix-free laser desorption/ionization mass spectrometry(LDI/MS). Four different kinds of NPG surfaces were prepared. The structures of NPG surfaces were controlled by applying different deposition charges during the formation of Ag-Au layers. As a result, each NPG surface contained different structures and different pore size of holes. The effect of the NPG surfaces were demonstrated by mass analysis of small molecules including verapamil hydrochloride, dexamethasone, and steroids. In our preliminary study, it was observed that the peak intensity is gradually increased as the pore size of the surface decreased. The small molecules were successfully analyzed without interference with matrix peaks in the low-mass range of the spectra. Thus, we expect NPG surfaces will be potentially useful for the analysis of small molecules by LDI/MS.

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Analysis of chondroitin sulfate in terms of matrix effects and quantitative determination by MALDI-TOF MS

신성재, 양효직, 김진희, 홍장미, 이선영, 김정권

충남대 화학과

Chondroitin sulfate (CS) is a complex polysaccharide, belonging to a family of glycosaminoglycans. CS consists of N-acetylgalactosamine disaccharide units. In this study, MALDI-TOF MS was used to quantitatively determine CS. Chondroitin ABC lyase was used for enzymatic digestion, generating N-acetylgalactosamine disaccharide units (M.W. = 503). In MALDI-TOF MS, the resulting disaccharides were observed as sodium adduct peaks at m/z 526. Different matrices such as 2,5-Dihydroxybenzoic acid (DHB), 2,6-DHB, and 2',4',6'-Trihydroxyacetophenone (THAP) were used to detect the disaccharides. Ionization efficiency and signal-to-noise ratio from THAP matrix were much better than those of the other matrices. Maltotriose (M.W. = 504) was used as an internal standard, providing a sodium adduct peak at m/z 527. Serial dilution (1~10-fold) of CS digest containing a constant amount of maltotriose was used to provide a calibration curve. The concentration of real sample of CS was determined by using the calibration curve which was obtained from the intensity ratio of the standard disaccharide of CS and maltotriose.

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Comparison of different columns in the analysis of carbohydrates

박세환, 신성재, 양효직, 김진희, 홍장미, 이선영, 김정권

충남대 화학과

AbstractThe performances of three different columns (Shodex NH2P-50 4E, HLC-A SPS 100-5, and NH2 SPS 100-5) which are frequently used in the analysis of carbohydrates were compared using five standard samples (N-Acetyl glucosamine, Glucosamine, Glucose, Mannose, and Sucrose). Isocratic elution was used to elute out sample using 50% Acetonitrile (ACN) or 75% ACN in water. The five standard samples were prepared in a concentration of 5 mg/ml (5000 ppm) in the LC solvent. UV and RI detectors were used for the detection of the carbohydrates. Adjusted retention time, retention time of unretained solute, retention time of solute of interest, intensity, W1/2, number of plates, and capacity factors were calculated based on the LC chromatograms. Each column has shown unique properties. In case of SiO2– based amine column (NH2 SPS 100-5), 50% ACN has to be used to elute out the carbohydrate in similar time scale from the other two columns using 75% ACN. Overall, Sio2-based amine column shows the best performance. The detailed experimental procedures and results will be provided during the presentation.

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Amperometric Proton Sensitive Sensors for Paraoxon Detection

Md. Mokarrom Hossain, Shaikh Nayeem Faisal, 이혜진

경북대 화학과

In this poster, we present an amperometric proton sensor that can selectively detect organophosphate pesticides (i.e., paraoxon). The sensing methodology is based on measuring the current change associated with the proton transfer by the proton selective ligand (e.g., ETH1778) across a micro-hole interface between the water and polyvinylchloride –2-nitrophenyloctylether gel phase. The selective detection of paraoxon using the proton sensor is achieved by measuring protons generated by the hydrolysis of paraoxon with the organophosphorus hydrolase (OPH) enzyme. The proton ion transfer reaction across the polarized micro-hole interface followed by the OPH enzyme reaction with paraoxon was fully characterized using cyclic voltammetry and differential pulse stripping voltammetry. The sensor exhibited good linear responses towards different concentrations of the paraoxon present in aqueous samples.

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Disk Sorptive Extraction Based on Monolithic Material Followed Gas Chromatography-Mass Spectrometry for the Analysis of Volatile Components from Vanilla

손현화, 이동선

서울여대 화학과

A disk type sorptive extraction using monolithic material (Mono Trap) based on silica bonded with octadecyl silane (ODS) and containing activated carbon was applied to the analysis of volatile components from vanilla perfume sample by gas chromatography-mass spectrometry (GC/MS). Several extractive parameters, including desorption solvent, adsorption temperature and time, solvent volume and sample volume were investigated in detailed and optimized. From the experimental results, the optimized parameters for the extraction of benzyl acetate, linalyl acetate, vanillin, and ethyl vanillin as the target compounds were the following: desorption solvent was 100 μL of dichloromethane using 30 μL of sample volume; extraction temperature and time were 60℃ and 90 min, respectively. Under the optimum conditions, detection limits (S/N=3) and quantification limits (S/N=10) of proposed method for the target compounds were achieved within the range of 8.35~13.7 6μg/mL and 27.82~45.88 μg/mL, respectively. The method showed good linearity with correlation coefficient more than 0.9888. The method was successfully applied to detect 11 volatile compounds from vanilla perfume with satisfactory recovery and reproducibility in the range of 81.20~ 90.24% and 1.18~2.85 RSD%, respectively. The results showed that disk sorptive extraction using Mono Trap is very simple and a new promising technique for the analysis of volatile aroma compounds from vanilla perfume.

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Electrochemical Determination of Hemoglobin A1c (HbA1c)

이정훈, *박종면, 최한님, 이원용

*연세대 화학과 *삼성종합기술원 바이오랩*

Diabetes, a disorder in the metabolism of glucose due to the lack or inability to use insulin to regulate the glucose level, is one of the major health concerns worldwide. Therefore, the monitoring of glucose level is necessary to diabetic patients. Glycated hemoglobin level has been used as one of the reliable markers of glycemic control. Glycated hemoglobin, which is called HbA1c, is formed by nonenzymatic glycosylation of hemoglobin exposed to high glucose levels in plasma. The detection of HbA1c is very important because it indicates the average blood glucose level over 3 months. In this study, we developed a sandwich type electrochemical sensor for the determination of HbA1c, which is based on the cis diol interaction between HbA1c and boronic acid. Detection of HbA1c was performed with simple procedure and technique. First, HbA1c was selectively bound into the self-assembled monolayer (SAM) of boronic acid on a gold electrode surface, and then electroactive ferrocene species containing boronic acid were bound into the opposite binding site of HbA1c to form a sandwich type complex. The HbA1c concentration was determined by cyclic voltammetry technique. The present sensor responded linearly to HbA1c in the wide concentration range from 0.0312 uM to 1.250 uM with a good sensitivity. Due to the binding selectivity of boronic acid in the sandwich type HbA1c sensor, the present electrochemical HbA1c sensor exhibited very good sensitivity. In addition, the present biosensor did not show any interference from excess of fructose and sorbitol. Furthermore, the HbA1c % in human plasma samples was successfully determined and compared to the result obtained with other methods. Therefore, the present sandwich type electrochemical HbA1c sensor might be applied for the determination of HbA1c in the human blood samples.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Determination of L-ascorbic Acid Using Silver Nanoparticles Sensitized Luminol-H_2O_2Chemiluminescence System

김소연, 타스리마펄도우스, 이상학, *김영호, 이성욱

*경북대 화학과 *경북대 차세대에너지기술연구소*

The determination of L-ascorbic acid by chemiluminescence (CL) method using silver nanoparticles has been studied. This method is based on increased chemiluminescence intensity with the addition of silver nanoparticles to the system of luminol and hydrogen peroxide, and it is based on the quenching of chemiluminescence intensity with addition of L-ascorbic acid. The effects of pH, concentrations of luminol, hydrogen peroxide and silver nanoparticles on the CL intensity were investigated. The CL intensity was measured at the 425 nm. A dramatical increase in intensity was detected when silver nanoparticles was added at the luminol and hydrogen peroxide system. When the L-ascorbic acid was added in the system, it decreased the CL intensity of the luminol- hydogenperoxide- siver nanoparticle system. The principal reason for quenching is likely to be the complex formation between L-ascorbic acid and silver nanoparticles. The calibration curve for L-ascorbic acid was linear over the range of 9.0×10^{-9}M to 2.9×10^{-7}M, the correction coefficient was 0.9997 and the detection limit was 3.5×10^{-9}M. The proposed method was applied to the determination of ascorbic acid in vitamin C tablets.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Functionalization of self-assembled monolayer on quartz plate by a covalently Bound tris(2-aminoethyl)amine based receptor for selective optical detection of zinc ion

김동완, 김재상

경상대 화학과

Surface reactions were employed to introduce a variety of functional groups in self-assembled mololayers (SAMs) on hydroxylated surfaces such as glass and quartz. The fluorescent receptors(I, II) were synthesized and immobilized quartz surface. The sensing ability was studied by addition of various metal cations to cuvett contain SAMs quartz plate. SAMs has been utilized as the basis of the fabrication of the Zn^{2+} sensitive fluorescent chemosensor. The analytical performance characteristics of the proposed Zn^{2+} chemosensor were investigated. The experiment results show excellent selectivity for $Zn2^{2+}$ over transition metal cations.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Development and testing standard compounds for quantitative analysis of crude oil

조윤주, *김성홍, 김성환

*경북대 화학과 *한국기초과학지원연구원 대구분소*

In this study, standard compounds for quantitative analysis of crude oil were synthesized and tested. Petroleum is one of the most complex materials in the world and there has been a lot of effort devoted to understand the chemical composition. Petroleomics, a new field of study, has been successfully used to study the composition of petroleum at a molecular level. In petroleomics, polar and heavy components of crude oil are qualitatively studied using ultrahigh-resolution mass spectrometry, particularly Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS). For the petroleomics to have more practical impact, it is very important to develop method for quantitative understanding of chemical components of petroleum. However, it has been difficult to do quantitative study due to lack of standard compounds. Compounds suitable for this kind of study were not commercially available. In our preliminary study, 9-hexadecyl, 9-octadecyl, 9-docosyl-9H-carbazole, and 2-hexadecylnaphthalene were synthesized. The compounds were confirmed by FAB-MS and NMR(400MHz). The compounds will be added to crude oil sample and analyzed by FT-ICR MS. More compounds including 2-octadecylnaphthalene and 2-hexadecylbenzothiopene will be synthesized and tested.

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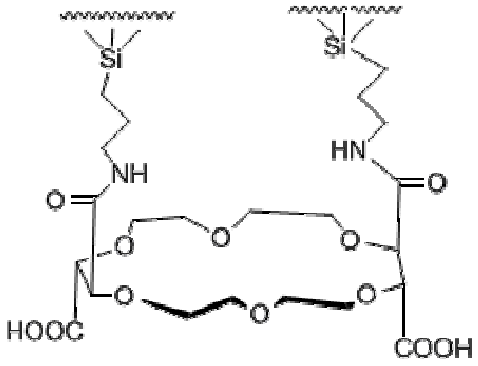
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

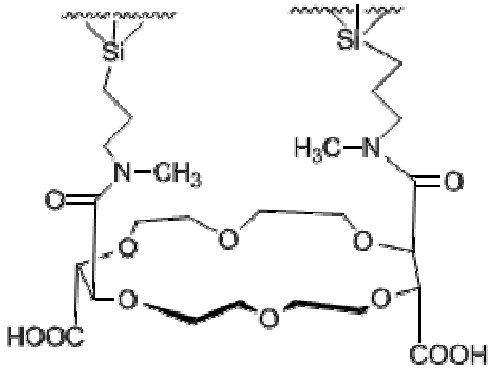
The Comparison of Enantiomeric Selectivity in Amino Acids Separation with Two type of Crown Ether-bonded Phase in High Performance Liquid Chromatography

진주현

(주)알에스텍

ChiroSil® (Fig.left) which is prepared by a covalent trifunctional bonding of (+)-(18-Crown-6)-tetracarboxylic acid on amino propyl silica gel have been proven that it is effective in resolving racemic amino acids, primary amines and amino alcohols[1]. The purpose of this study is to determine and compare enantioselectivity of ChiroSil® and ChiroSil-M® (Fig.right) which is newly developed and simply prepared by substituting N–H hydrogens of the tethering groups of ChiroSil® for methyl groups[2-4]. To compare with ChiroSil® and ChiroSil-M®, retention and chiral selectivity data using HPLC were measured in mobile phases of varying acidic modifier, composition of organic modifier and temperature for primary amino acids. In experimental results, ChiroSil® and ChiroSil-M® showed complementary chiral recognition behavior in amino acids resolution under the various mobile phase conditions adjusting organic concentration and changing acidic modifier. We analyzed the thermodynamics property of selected amino acids from the mobile phase to the chiral stationary ChiroSil® and ChiroSil-M® in reversed-phase HPLC. This type of anaylsis is performed by applying a form of the Van't Hoff equation[5]. The result will be discussed. Consequently, the chiral recognition mechanism on these two columns was presumed to be different and the combination use of these two columns can be one of the solutions to more satisfied resolution in amino acids separation. [1] M.H. Hyun, J. S. Jin, W. Lee, J. Chromatogr. A. 1998, 822(1), 155.[2] M.H. Hyun, Y. J. Jin, J. S. Jin, J. Chromatogr. A. 2003, 984(2), 163.[3] M.H. Hyun, Y. J. Cho, J. A. Kim, J. S. Jin, J. Liq.Chromatogr. Rel. Technol. 2003, 26, 1083[4] M.H. Hyun, G. Tan, Y. J. Cho, J. Liq. Chromatogr. Rel. Technol. 2004, 27, 1671.[5] T. L. Chester, J.W. Coym, J. Chromatogr. A. 2003, 1003, 101.





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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Selective separation of Be^{2+} by supported liquid membranes (SLMs) containing 1,4-benzodioxan derivatives

이은빈, 김동완, 김재상

경상대 화학과

In this study, 1,4-benzodioxan derivatives L^1,L^2 and L^3 were synthesized and studied as ditopic L^1 and monotopic carriers L^2,L^3 for liquid membrane transport of Be^{2+} and various ions. The SLMs transport studies used a liquid membrane of plasticizer (NPOE,TEHP) supported by a thin and flat PVC. Various parameters like feed acidity, carrier concentration, and membrane thickness was investigated and optimized. Especially, membranes containing ditopic carriers, L^1 exhibited an excellently selective and effective transporting ability for Be^{2+}.

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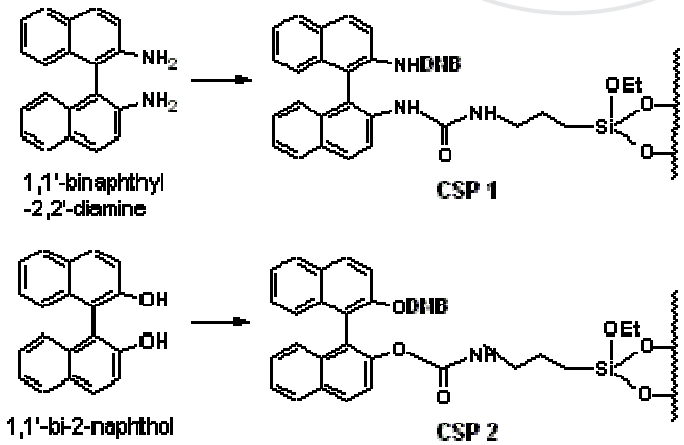
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Enantioseparation of various racemic compounds on Binaphthyldiamine and Binaphthol 3,5-Dinitrobenzoyl derivative Chiral Stationary Phases

유정재, *Yi Zun Zhang, **류재정

*경북대 사범대 화학교육과 *Henan Institute of Science and Technology **경북대 화학교육과*

Recently, 1,1'- binaphthyl-2,2'-diamine 3,5-dinitrobenzoyl derivative chiral stationary phase (CSP 1) was prepared and used for chiral separation of eleven chiral compounds.[1] In this study, the preparation of a 1,1'-bi-2-naphthol 3,5-dinitrobenzoyl derivative chiral stationary phase (CSP 2) and application of the CSPs for the separation of more than 20 chiral compounds will be shown. For exact comparison between CSP 1 and CSP 2, we prepared the CSP 1 again under the same synthetic condition of CSP 2.1) J.J. Ryoo, J.J.; Armstrong, D.W. Bull.Korean Chem. Soc. 2007, 28, 2103.



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The stability of cupper with hydrotalcite by deposition, using electrolysis

김태호, 김이영, 김지혜, 나성옥, 최보라, 김종원, 정용석, 권수한

충북대 화학과

본 연구는 전기분해를 이용하여 하이드로탈사이트에 구리이온을 침착시키는 것을 목적으로 한다. 전기분해 장치를 이용해 구리판에서 구리이온을 얻어 침착시키는 것으로 반응시간, 온도, pH, 전압을 변화시켜 반응성을 알아보고 나타난 결과를 보고 반응이 일어나는 최적조건을 찾는다. 또한 그 생성된 물질과 기존 물질의 안정성을 테스트해보고 유용한 물질을 찾아낸다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Determination of L-Phenylalanine Using Luminol-H_2O_2-Cu^{2+} Chemiluminescence System Coupled with Flow Injection Analysis

타스리마펄도우스, 이상학, *최종하, 조해진, 이성욱

*경북대 화학과 *안동대 화학과*

A highly sensitive flow-injection chemiluminescence (CL) method for the determination of L-phenylalanine (L-PA) has been developed. Proposed method is based on the enhancement effect of L-PA on the chemiluminescence signals of luminol-H_2O_2-Cu^{2+} system in alkaline medium. The optimum condition for the CL reaction was studied in detail using flow-injection system. The experiments indicated that under optimum condition, the CL intensity was linearly related to the concentration of L-PA in the range of 5.2×10^{-9} – 1.9×10^{-6} mol L^{-1} with a detection limit (3σ) of 2.8×10^{-9} mol L^{-1}. The proposed method had good reproducibility with the relative standard deviation (RSD, n=7) of 2.0 % for 1×10^{-8} mol L^{-1} of L-PA. This method has the advantages of simple operation, fast response and high sensitivity. The possible mechanism of the CL reaction is discussed based on the kinetic characteristics, CL spectra and UV spectra. The proposed method was successfully applied for the determination of L-PA in diet soft drinks and also in pharmaceutical preparations.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Flow Injection Chemiluminescence Determination of a Triazine Compound Using Luminol and Silver Nanoparticles

타스리마펼도우스, 이상학, *최종하, 조해진

*경북대 화학과 *안동대 화학과*

The effect of silver colloidal nanoparticles (AgNPs) on melamine, triazine compound, was investigated using flow injection chemiluminescence system. It was found that AgNPs could act as a nanocatalyst on the luminol– melamine system to generate chemiluminescence (CL). The CL emission spectrum of the luminol– melamine –AgNPs system showed a peak with a maximum at 425 nm. It was suggested that the luminophor species was the excited state 3-aminophthalate. The reduction of dissolved O_2 to H_2O_2 by melamine and decomposition of H_2O_2 to the oxygen-related radicals were attributed to the catalytic effect of AgNPs. Under optimized conditions, the CL signal intensity was linear with the melamine concentration in the range range of 5.5×10^{-9} – 1.8×10^{-6} mol L^{-1} with the correlation coefficient of 0.9996. The limit of detection was 3.4×10^{-9}mol L^{-1} melamine. The relative standard deviation for seven repeated measurements of 1.0×10^{-7} mol L^{-1} melamine was 1.5%.The effect of potent interfering compounds on the CL signal intensity of the proposed luminol– melamine–AgNPs system was investigated. The proposed method was successfully applied to the determination of melamine in milk sample.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Detection of explosive materials using the SPR technique based on the molecular imprinted polymer(MIP) films

양승주, 조영호, 유연규, *박찬량

*국민대 생명나노화학과 *국민대 화학과*

Gas phase detection of the explosive materials(TNT, DNT, NT) was studied utilizing the surface plasmon resonance phenomena. The molecularly imprinted polymers(MIP) were prepared using the thermal polymerization method and coated as a sensing layer on the Au surface. The morphology of the films were measured using SEM and AFM. The detection limit of the MIP-based SPR sensor was obtained at the level of about several tens of ppb. The sensitivity dependence on the various synthesis conditions of MIP films were measured and interpreted on the basis of structural difference of the polymer films. The selectivity test against toluene vapor was also accomplished and compared with other results.

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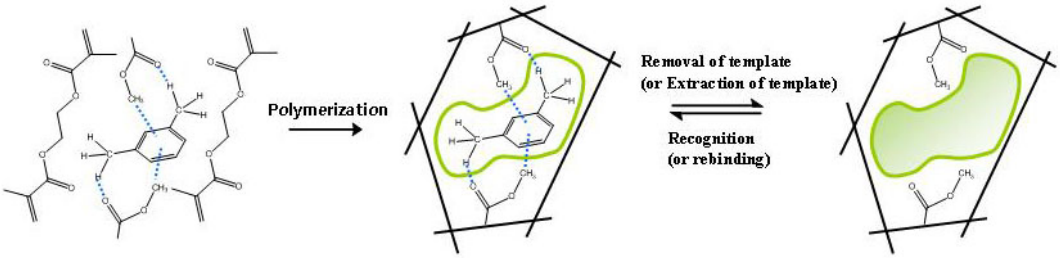
발표종류: 포스터, 발표일시: 금 15:00~17:00

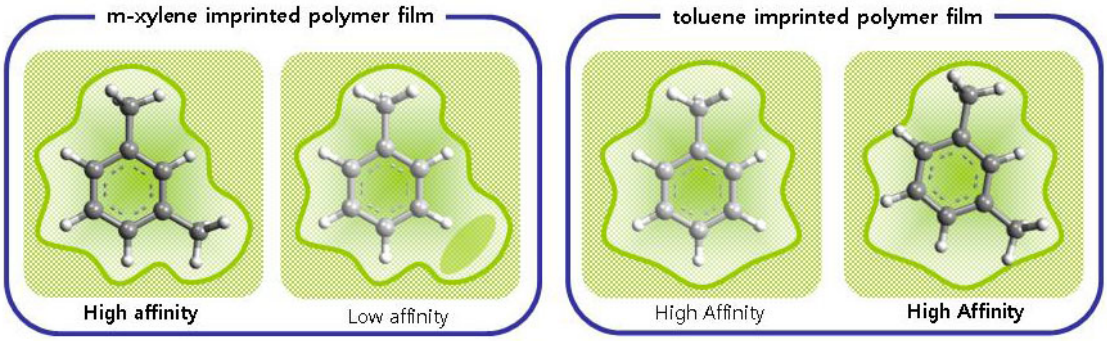
Molecularly imprinted polymer thin films for analysis of gaseous m-xylene and toluene using surface plasmon resonance technique

장성우, *도영락, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We applied molecularly imprinted polymer thin films to the sensing of gaseous m-xylene and toluene using SPR technique. The molecularly imprinted polymer films were synthesized by UV-induced polymerization method using several different functional monomers. The morphologies of polymer films were obtained by atomic force microscopy at various thicknesses. The detection limit of the MIP films for m-xylene and toluene was obtained at several ppb level and the selectivity of the m-xylene-imprinted polymer were tested against the humidity, formaldehyde, ammonia and toluene. The association and dissociation curves of the sensorgrams for the m-xylene-imprinted polymer films were fitted using the conventional kinetic models, and the homogeneity of imprinted polymer film were characterized using Langmuir-Freundlich isotherm model. Additionally the interactions between template(m-xylene) and imprinted polymer films were measured using FT-IR spectroscopy with single ATR technique.





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발표종류: 포스터, 발표일시: 금 15:00~17:00

Liquid chromatographic resolution of α –amino acids on a new ligand exchange chiral stationary phase (CSP) derived from leucinol

하진주, 마동희, 박수현, 현명호

부산대 화학과

A new ligand exchange chiral stationary phase (CSP) has been developed by covalently bonding (S)-N,N-carboxymethyl undecyl leucinol mono-sodium salt and octyltriethoxysilane onto silica gel and applied to the resolution of α-amino acids. In the resolution of α-amino acids, the new CSP was better in terms of the separation factors (α) and the resolution factors (Rs) in most of cases than the old one which was previously developed by covalently bonding (S)-N,N-carboxymethyl undecyl leucinol mono-sodium salt onto silica gel. The chromatographic resolution behaviors were dependent on the type and the content of organic modifier and Cu(II) concentration in aqueous mobile phase.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

HPLC resolution of racemic mexiletine analogues on chiral stationary phase based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid

진갑봉, 한혜지, 현명호

부산대 화학과

Mexiletine is an effective sodium channel blocker used as an antiarrhythmic and analgesic oral drug. Structure activity studies in vivo and in vitro of pharmacologically active mexiletine indicate that (-)-(R)-mexiletine binds preferentially to the cardiac sodium channels. In addition, (-)-(R)-mexiletine is also more active than (+)-(S)-mexiletine on native skeletal muscular fibers. The use of mexiletine as a racemate in the treatment of neuromuscular disorders is limited due to its possible side effects.In this study, we prepared various mexiletine analogues and resolved them on a chiral stationary phase based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid. Resolution of the mexiletine analogues on the chiral stationary phase based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid was found to be dependent on the mobile phase compositions.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Liquid chromatographic resolution of α- amino acids on a new ligand exchange chiral stationary phase (CSP) derived from phenylglycinol

마동희, 하진주, 현명호

부산대 화학과

The resolution of racemic compounds has been considered as one of the difficult problems in separation science. But, recently liquid chromatography resolution of racemic compounds on chiral stationary phases (CSP) has been studied by many works in area of organic chemistry, medical science and pharmacological studies. Chiral ligand exchange liquid chromatography has been reported to be a powerful technique for the resolution of racemic amino acids. In this study, a new ligand exchange stationary phase (CSP) was developed by covalently bonding (R)-N,N-carboxymethyl undecyl phenylglycinol mono-sodium salt and octyltriethoxysilane onto silica gel. The CSP developed in this study was applied to the resolution of α-amino acids. The new CSP was much better in terms of the resolution factors (Rs) and separationfactors (α) than the old one developed previously by covalently bonding (R)-N,N-carboxymethyl undecyl phenylglycinol mono-sodium salt onto silica gel in terms of the resolution factors (Rs) and separationfactors (α). In an effort to characterize the new CSP, the chromatographic behaviors for the resolution of selected α-amino acids were investigated with the variation of the content of organic modifier and Cu(Ⅱ) concentration in aqueous mobile phase.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Enzymeless electrochemical detection of Hydrogen peroxide

박초롱, 김혁한, 최영봉

단국대 화학과

Simple and reliable measurements of hydrogen peroxide have been continued to receive considerable attention particularly in physiological, biomedical and environmental studies, with many applications found in the food processing, pharmaceutical industry, etc. Hydrogen peroxide has been proven as a key reactive oxygen species in plant cells hence its measurement in plant samples is of particular significance. It is also a by-product of many biological oxidative reactions, e.g., glucose oxidase/glucose and other oxidases, therefore it is an very important parameter for monitoring biological processes. Extensive studies of hydrogen peroxide (H2O2) have been done using horseradish peroxidase (HRP) that catalyzes hydrogen peroxide to water. Although enzymatic detection usually shows good selectivity and sensitivity, the activity of enzyme is easily decreased during its immobilization process. In this work we propose the detection of hydrogen peroxide with different Os & Ru mediators without horseradish peroxidase (HRP). These experimental facts showed that enzymeless H2O2 sensor is one of a promising tools to develop a hydrogen peroxide sensor.

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Preparation of antibody hippuric acid-modified magnetic beads and its application of an amperometric immunosensor

전원용, 최영봉, 김혁한

단국대 화학과

Urinary hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. The urinary HA 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 electro chemical 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 (Ag-HA-Os) complex was prepared and then characterized using electrochemical techniques. The electrochemical immunoassay comprised antibody-HA-magnetic beads and then applied to mixture of HA-Os and hippuric acid (HA) in the micro-tube. By magnetic beads after separation, then the electrical signals were measured by voltammetry technique. The resulting currents were linearly related with the concentration of antigen HA through the competitive reaction between HA-Os and HA. A study of the electrochemical immunoassay offer the development of cheap, miniature devices capable of performing rapid immunoassays.

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Characterisation of an Optical Sensor for Determination of Zn(II) and Cu(II) Using Homo-Ditopic Receptors

김관겸, 김동완, 김재상

경상대 화학과

An fluorescent optical sensor based on a exchange mechanism for the determination of Zn(II) and Cu(II) has been developed. The optode membrane is constructed by immobilization of homoditopic salophene as senor element on plasticizer/PVC membrane. The exchange of proton of salophen schiff's base in the membrane interface with various metal ions was monitored Uv-Vis. And spectrofluorometry. The change in the absorbance of the membrane was used for determination of mtal concentration. The parameters, such as pH, membrane thickness, concentration and composition, linear range, detection limit were optimized . The proposed sensor was successfully applied for the determination of Zn(II) in real samples.

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Chlorine degradation and discoloration of Polyurethane

박민경, 오종하, 홍지혜, 이귤섭

(주)효성

Hypochlorite, considered as one of the strongest oxidizing agent, deteriorates the properties of polyurethane by causing its degradation and discoloration. In this report, we suggest that hypochlorite cleaves urethane bond of polyurethane, making 4,4'-methylenedibenzenamine and some of that turn into 4,4'-methylenebis(2-chlorobenzenamine) through ring chlorination. These yellow byproducts are the main cause of discoloration of polyurethane. Furthermore, we reveal that metals such as Al and Fe generally used as an anti-chlorine agent catalyze ring chlorination. This study reports the plausible mechanism about how the structure of polyurethane changes in NaOCl, by using ATR-IR, NMR and GC/MS.

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Preparation of C18 modified monolithic silica particles and their application in HPLC

이주영, 정원조

인하대 화학과

This work demonstrates the chromatographic separation performance of a microcolumn packed with C18 modified monolithic silica particles. Most researchers are making stationary phases by using commercial silica particles because of their stability and good separation efficiency. We prepared a new type of stationary phase of improved stability and separation efficiency. A specific reaction mixture of TMOS (tetramethylorthosilicate), PEG(polyethylene glycol), Urea, and acetic acid was prepared in a vial and heated to form silica monolith. The silica monolith was ground into fine particles of ca 2.5 um average size. These particles were modified with a C18 ligand, end-capped, and packed in a microcolumn. This column showed quite good separation efficiency and it was even superior to the microcolumn packed with a commercial spherical C18 stationary phase.

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Determination of analytical methods for organotin compounds using liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICP-MS) and electro-spray ionization mass spectrometry (ESI-MS) as complementary techniques

이우영, *이경석, *임용현, *임영란, **김태규, *황의진

*부산대 물리화학 *한국표준과학연구원 분석화학표준센터 **부산대 화학과*

Since organotin compounds such as monobutyltin (MBT), dibutyltin (DBT), and tributyltin (TBT), are very toxic even at low concentration comparing with elemental tin, the use of these compounds are strictly limited by international organizations such as the International Marine Organization (IMO). However, these compounds and their metabolites still can be detected in waters, sediments, and, even, foods. Therefore, it is important to develop accurate analytical methods for quantitative determination of these compounds. In this study, analytical methods for monobutyltin (MBT), dibutyltin (DBT), and tributyltin (TBT) have been developed using liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICP/MS) and electro-spray ionization mass spectrometry (ESI-MS). As results, we found compatible separation conditions for both techniques and optimized the experimental conditions for the best performance. Though LC-ICP/MS provides excellent sensitivity, selectivity, and wide linear dynamic range, it generally gives limited information about each chemical structure. On the other hand, LC-MS has advantages to obtain detailed structural information for each species so that it can be a good complementary method for organotin speciation analysis.

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Quantitiative evaluation of chitooligosaccharide and fructooligosaccharide by MALDI-TOF MS

김진희, 양효직, 신성재, 홍장미, 이선영, 박세환, 김정권

충남대 화학과

Chitooligosaccharide is a kind of oligosaccharide which is made from chitin or chitosan by chemical or enzymatic decomposing method. With its excellent physiological activity and function it has wide usage. Fructooligosaccharide is a complex sugar derived from plants and is very good for the human body in contrast to the commonly used refined sugar. The complex sugar is even marketed nowadays as nutritional supplements as it is so healthy and has so many beneficial effects. In this study, Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) was successfully applied to quantitatively analyze chitooligosaccharide and fructooligosaccharide. Standard oligosaccharides with nystose as an internal standard were used to generate calibration curves. For the analysis of chitooligosaccharide, the intensity ratios of G4 (m/z 685.6) and nystose (m/z 689.6) were utilized for quantitation. For the analysis of fructooligosaccharide, standard addition of constant amount of nystose to various amount of fructooligosaccharide were used for quantitiation where the change of GF3 intensity was used for quantitiative information. Real samples from the market were also analyzed by the current method.

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Shotgun Lipidomics of Lipid Extract from Mouse Brain

박태성, 김영환

한국기초과학지원연구원 질량분석연구부

Lipids are essential cellular constituents that are multiple distinct yet critical roles as membrane bilayer, reservoirs for energy storage and the source of second messengers, in cellular function. The unique chemical structure of the majority of lipid molecular specie consists of linear combination of a small number of building blocks that inclued backbones, head groups, and aliphatic chains. Recently, shotgun-lipidomics, to direct qualitative and quantitative analysis of complex mixtures of lipid by mass spectrometry have defined large-scale study of the pathways and networks of cellular lipids, is a newly and rapidly expanding research field in system biology. In this study, we analyzed glycero-phospholipids and sphingolipids at molecular level that extracted in normal mouse brain by using methyl-tert-butyl ether (MTBE). The high resolution mass spectra using 15T-FT-ICR mass spectrometer provide profiling of lipid extract in mouse brain. Each lipid class was characterized by intra-source separation method. Because the majority of lipid classes possess a unique fragment ions resulting from the head group and aliphatic chains after collision-induced dissociation (CID), precursor ion scan or neutral loss scan was employed to identify the individual molecular species using triple quadrupole mass spectrometry.

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A discrimination between polarimeter and chiral HPLC for the determination of optical purity of (L)-amino acids

이미성, *김태규, 오채영, **문해경, ***정의덕, ***진종성

*부산대 화학과 *한국기초과학지원연구원 **한국기초과학지원연구원 하이테크소재연구부 ***한국기초과학지원연구원 하이테크부품소재연구지원센터*

Although an assay method for the content of amino acids is provided as titration which could not distinguish (L)-amino acid with (D)-amino acid, definitions of content are expressed as (L)-amino acid in the KP* and USP* . We want to confirm the relation of scope between content and specific rotation (α) using the methods in the KP and USP. On the other hand, we want to compare specific rotation (α) using polarimeter with enantiomeric excess (ee) using chiral crown ether HPLC column for (L)-amino acids. And we find out m/z of the front peak on the chromatogram from LC/MS/MS whether amino acid becomes degradation.{* KP : Korean Pharmacopeia, * USP : United States Pharmacopeia}

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Fluorescence stability test of FITC in FITC doped silica BEADs for biological application

고정아, 임홍빈

단국대 화학과

Many biological experiments (especially at molecular level) have been importantly progressed using various tools of imaging or detection. Among the many developed analytical tools, fluorescence spectrometry is the most frequently used method because it is easy to control and highly selective and sensitive than other method. But there are some problems to be solved like photobleaching and quenching, in other words fluorescence intensity was reduced by several factors. In order to solve these problems, we synthesize a dye doped silica nanoparticle with a protection layer with TEOS (so called “core-shell nanoparticle”), then studied the photostability of FITC.For quantitative detection, we use a lab-built laser induced fluorescence microscope (LIFM) with Photomultiplier tube(PMT) and 473nm DPSS Laser(with 500nm~550nm interference filter). After irradiating laser beam for an hour, fluorescence suppression was observed for FITC in solution and the core-shell nanoparticle. As a result, both fluorescence intensities were suppressed, but the core-shell nanoparticle showed 10% signal reduction, while FITC in solution showed about 90%. Furthermore, quenching strength by various metal ions (Na+, K+, Ca2+, Mg2+, Pb2+, Cd2+, Hg2+) on the nanoparticle depended upon the hydrated ionic size. For instance, singly charged ions showed almost no quenching whereas divalent metal ions suppressed the fluorescence even for the nanoparticle with silica protection layer.

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Examination of template structural effects on CEC chiral separation performance of molecule imprinted polymer made by a generalized preparation protocol

shabiabbas, 정원조

인하대 화학과

Some acidic chiral templates were used to prepare open tubular (OT) molecule imprinted polymer (MIP) capillary columns to explore the effects of molecular structures of templates on chiral recognition capabilities and to verify the feasibility of the general MIP preparation protocol introduced in the previous study. The templates are phenyl carboxylic acids and their derivatives. Optimization was carried out for chiral separation of template enantiomers for each MIP column through varying pH and composition of eluent. It was found that the preparation protocol can be successfully applied for the appropriate templates with functional groups fulfilling the 3-points interaction rule. The chiral separation performances were quite satisfactory for MIPs of such templates although they are yet inferior to the separation performances of the MIP columns fabricated with the templates of profen drugs (2-arylpropionic acids with a large substituent on the phenyl ring). Subtle variations of the template molecular structures have been found to be critical to enhance chiral recognition ability of the resultant MIP column.

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Detection of biomarker tagged with highly selective heavy metal using LA-ICP-MS

윤수영, 임홍빈

단국대 화학과

Recently, quantification of bio materials has becoming important for pathogenic diagnosis. Fluorescence detection tagged to the bio materials was commonly applied to the diagnosis. However it had some disadvantages that had less bio molecular fluorescence and high interference. Determination of highly selective heavy metal tagged bio-marker using Inductively Coupled Plasma Mass Spectrometry (ICP-MS) was a highly sensitive and almost interference-free technique, compared to bio molecular fluorescence. Particularly, laser ablation sampling in ICP-MS required a small sample volume. In addition, we developed a picoliter sampling using polydimethylsiloxane microarray chip (PDMS microarray chip). In this experiment, a detection system of IgG immobilized on a PDMS microarray chip was developed using Gd complex for bio-tagging. For the preparation of Gd-complex, the solution of p-NH2-Bn-1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (p-NH2-Bn-DOTA) 32ppm and Gd 100ppm was mixed and autoclaved for 30min at 120℃. The unreacted free Gd was removed by the catex column, of which the process showed the yield of 56.9% for Gd complex. For the immobilization of IgG on the PDMS chip, epoxy was coated by chemical vapor deposition method. The mixture of Immunoglobulin G (IgG) and PBS buffer solution was loaded on the epoxy treated PDMS-island chip in the incubator for 24 hours. The unreacted the mixture of IgG matrix washed out by PBS buffer solution and then the complex of Gd solution was loaded on the IgG modified PDMS chip in the incubator for 24 hours. The concentration of Gd on the PDMS pillar was determined by LA-ICP-MS. In this experiment, calibration curve was obtained with the linear regression coefficient, R2, of 0.974. This method can be applied for development of clinical diagnosis.

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Synthesis of titanium dioxide nanoparticles for high dispersion and size control

김종민, 임홍빈

단국대 화학과

Titanium nanoparticles are widely used in various industrial fields, for dye, paint, sun block, photo catalysis, etc. But the most common issues for application are particle size and dispersion. This experiment conducts synthesis of amorphous nano size titanium particles that has small size and high dispersion due to large surface area. To synthesis the monodispersed titania nanoparticle, titanium tetraisopropoxide and ammonia were used as a source and catalyst, respectively. After optimizing the synthetic condition by taking the amount of TTIP, ammonia, stirring speed, and reaction time at room temperature into consideration, the particle size was controlled by polymer binder, which played the role of surfactant, formed micelle with titanium nanoparticle, and prevented from the particle growing. The synthesized titanium dioxide was characterized by Field Emission Scanning Electron Microscope (FE-SEM) and X-ray Diffraction (XRD), for the particle size distribution and crystallinity. The dispersivity of the nanoparticles was also observed and comparted with commercialized titanium dioxides used for pigment in dye.

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Determination of Ceruloplasmin in Serum using LA-ICP-MS

주재영, *임홍빈

*단국대 자연과학부 화학과 *단국대 화학과*

Ceruloplasmin is the major copper-carrying protein in the blood. Lower-than-normal ceruloplasmin levels may indicate Menkes disease, Wilson's disease, etc and greater-than-normal ceruloplasmin levels may indicate or be noticed in lymphoma, rheumatoid arthritis, Alzheimer's disease, etc. Although many detection methods for bio-samples have been studied in these days, such as fluorescence that shows extremely high sensitivity and selectivity if properly tagged, it has some drawbacks to get quantitative figures for ceruloplasmin. Furthermore, limited sample volume could restrict the choice of analytical methods because most of bio samples are taken from living organism. In this experiment, laser ablation (LA)-ICP-MS is employed to determine ceruloplasmin in serum by detecting Cu owing to stoichiometric binding of a ceruloplasmin with six Cu ions. One of the advantages of the laser ablation for sampling is small sample volume and direct analysis with less contamination. Particularly, we already developed and reported picoliter sampling technique for LA-ICP-MS. For sampling, PDMS mask was made with polyethyleneterephthalate film. 3x3 arrayed 150μm-diameter-PDMS pillars were made and treated with oxygen plasma. After then, 3-Glycidoxypropyl-trimethoxysilane was reacted with pillar surfaces to immobilize ceruloplasmin antibody (IgG) for a day. For bio application, serums of cancer patients were loaded on each island and reacted for a day. Because ceruloplasmin binds specifically with ceruloplasmin antibody through antigen-antibody reaction, ceruloplasmin will remain on the pillar after washing with PBS buffer. The concentration of ceruloplasmin was estimated from the concentration of Cu on the microarray chip determined by LA-ICP-MS. Calibration curve with the linear regression coefficient of 0.998 was obtained using commercialized human ceruloplasmin standards.

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Synthesis of NI-Al-Mg hydrotalcite compound by using the urea hydrolysis reaction

최보라, 김이영, 김지혜, 김태호, 나성옥, 권수한, 김종원, 정용석

충북대 화학과

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대한화학회 THE KOREAN CHEMICAL SOCIETY

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Separation of Aluminum Etchant using Capillary electrophoresis

장정우, *임홍빈, **성용익

*단국대 분석화학 *단국대 화학과 **단국대 개발부*

Liquid crystal display(LCD) manufacturing processes require various chemicals. To improve the yield and decrease the defects, concentrations of each constituent must be determined and controlled. Aluminum etchant is most frequently used to aluminum etching process of LCD manufacturing. It is composed of Phosphate, Nitrate, Acetate, and some salts. At this point, accurate process control of etching rate and depth can be done by controlling the concentration of each chemical. Monitoring of trace impurities is also required to control the process and recycle waste materials. However, existing analytical methods is too complicated and requires long analysis time. Furthermore, reliable analytical methods to determine acetate and some salts have not been developed yet. In this study, determination of the components in the etchant was demonstrated using capillary electrophoresis(CE). Since anions and cation can be determined by CE with small amount of sample and in a short time, some anions such as acetate, nitrate, and phosphate, and a cation, such as ammonium, in aluminum etchant were separated simultaneously using capillary zone electrophoresis(CZE) with indirect detection mode. The anion kit and cation kit from Beckman coulter were used as electrolytes. The detection limits for each ingredient were in the range from 19 to 1747ug. The relative standard deviations (n=4) of the method were between 0.35% and 6.05% for peak areas. Additionally, this optimized CE method was demonstrated for the analysis of different types of Al etchant used in the process.

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SERS imaging of VEGF-overexpressed breast cancer cells using aptamer-conjugated Au/Ag core/shell nanoparticles

고주희, 이상엽, *주재범

*한양대 응용화학과 *한양대 바이오나노공학과*

In this study, a novel detection method for VEGF biomarker targets, using aptamer/gold-core silver-shell nanoparticle bioconjugates, has been developed. This approach shows a high sensitivity, specificity and stability compared to conventional marker detection technologies. To apply SERS-based imaging technology, Raman reporter-labeled Au/Ag core/shell nanoparticles were fabricated and specific aptamer molecules were conjugated on their surface for specific targeting of VEGF markers overexpressed in breast cancer cells. The SERS intensities of Raman reporter are changed with the concentration variation of VEGF and this can be used for its localized distribution in breast cancer cells. This makes the SERS imaging technique using aptamer-conjugated functional nanoparticles potentially useful in early cancer diagnosis.

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The antioxidanive activity of leaves and fruit spine shell Castanea crenata var dulcis

주성진, *신장철, 김일광

*원광대 생명나노화학부 *원광대 화학과*

Leaves and fruit spine shell Castanea crenata var dulcis were extracted with pressurized methanol (80%), then fractionated with n-hexane, ethyl acetate (EA), butyl alcohol (BuOH), and H2O. The antioxidant capabilities of the samples were determined by following methods: free radical scavenging test (1,1diphenyl-2- picryl-hydrazyl DPPH), reductive potential method, and total phenolics method, total flavonoid. The antioxidant activities for extracts of leaves and fruit spine shell were compared to control antioxidants such as butylated hydroxyanisol (BHA), butylated hydroxytoluene(BHT), and a-tocopherol. The compounds activity of the leaves extracts were procyanidins, quercecetin, catechtin, and polyhydroxy phenols, and showed a good effect for antioxidant activity and MTT test.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Analyzed the saturated and unsaturated fatty acid of some nonvegetable foods by GCMS-QP2100

신장철, *주성진, *김일광

*원광대 화학과 *원광대 생명나노화학부*

Some nonvegetable foods as chicken, milk, egg, hairtail, cuttlefish and clam were dried in vacuum freeze-drying and the total fat were extracted with ethyl ether by a soxhlet fat extracting equipment. The saturated (SFA) and unsaturated (USFA) fatty acid in the curde fat was derivatized by boron triflouride diethyl etherate (BTDE) and analyzied with GCMS-QP2100. Finally the quantitative of the fat, SFA and USFA were calculated with peak area that showed on gas chromatogram spectro, the qualitative analysis were base on the similarity search mass spectro in the WILEY 8. library and compared with fatty acid methyl esters standard.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

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발표코드: **ANAL.P-60**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

A study about stability of Ti-hydrotalcite synthesis from electrolytic decomposition process

김지혜, 김이영, 김태호, 나성옥, 최보라, 김종원, 정용석, 권수한

충북대 화학과

본 연구는 전기분해를 이용하여 티타늄을 하이드로탈사이트 표면에 침착시켜 Ti-하이드로탈사이트를 합성시키는 것을 토대로 한다. 전압, 농도는 최적조건에 맞춰 합성하고 반응하는 시간에 따라 티타늄이 하이드로탈사이트에 침착되는 정도를 알아본다. 생성된 Ti-하이드로탈사이트는 응용하여 사용할 수 있는 물질인지 안정성을 테스트 해본다. 본연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Micelle-Sensitized Determination of Gatifloxacin in Pharmaceutical Preparations and Spiked Urine by Flow Injection Chemiluminescence Method using Ce(IV)-$Na_2S_2O_3$System

MD.KAMRUZZAMAN, *타스리마펄도우스, *이상학

*경북대 화학과 분광분석 실험실 *경북대 화학과*

A simple, sensitive and rapid flow-injection chemiluminescence (CL) method has been developed for the determination of gatifloxacin in pharmaceutical preparations and human urine. The method is based on the enhancing effect of gatifloxacin on CL emission generated by sodium thiosulphate and Ce(IV) in sulphuric acid sensitized by sodium dodecyl benzene sulfonate (SDBS). Strong CL emission was observed when gatifloxacin was injected into the Ce(IV) in sulfuric acid and $Na_2S_2O_3$ solution incorporated with SDBS in a flow-cell. Different experimental parameters affecting the CL reaction were studied and optimized systematically. Under the optimum conditions, it was found that the CL intensity is proportional to the concentration of gatifloxacin in the range of 1.10×10^{-10}-4.36×10^{-8} g mL^{-1} with a co-relation coefficient of 0.9993. The limit of detection (LOD) as defined by IUPAC (C_{LOD} =3×Sb/m, where Sb is the standard deviation of the blank signals and m is the slope of the calibration graph) was found to be 2.33×10^{-11}g mL^{-1} the relative standard deviation (RSD, n=7) was 1.41 % for 2.4×10^{-8} g mL^{-1} of GFLX. The proposed method does not require sophisticated instrumentation which offers higher sensitivity, wider linear range and better stability. Thus, the proposed method has been successfully applied to the determination of gatifloxacin in pharmaceuticals and human urine.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Encapsulation process of alginate-silicate hybrid polymer

강상혁, 김진산, 팽기정

연세대 화학과

Alginate is a natural bio-polymer of metal state of alginic acid that can be extracted from brown algae(Undaria pinnatiofida). These natural polymers are very abundant in ocean, non toxic to human body and show high chemical stability. But alginates have high viscosity and are hard to control. To solve these problems, we hybridized alginate and silicate for encapsulation that classified type of drug delivery system (DDS). Alginate hybrid (micro size bead form) can be prepared from a sodium alginate using calcium chloride as a cross-linker. We were varying sodium alginate, cross-linker solution's concentrations. The blank and alginate hybrid copolymer beads were characterized by using Fourier transform infrared spectroscopy (FT-IR), scanning electron microscope (SEM), porosity, thermo gravimetric analysis (TGA) and Thermogravimetric Analyzer (TGA). Surface morphology changes by changing the cross-linker, cross-linker concentration and various solvent compositions at same magnification. Total intrusion volume, porosity (%) and pore size distribution also change by changing cross-linker and cross-linker concentration. We also encapsulated some water soluble nutrients. And amounts of released nutrient are detected by Liquid Chromatography system.

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Reduction of perchlorate in water using stabilized nanoscale zero-valent iron particles

주태경, 김진산, 박수민, 강상혁, 팽기정

연세대 화학과

Perchlorate (ClO_4^-) has been widely used as oxidizing agent in military weapon system such as rocket and missile fuel propellant. Recently, it has been detected in the groundwater and considered as contaminant. Because perchlorate is known for its bad influence on human health, it has been challenging to remove and reuse the perchlorate. The many treatment technics for perchlorate have been developed such as adsorption, electrodialysis, bioreduction, and catalytic reduction. In this study, we focused on catalytic reduction of perchlorate by nanoscale zero-valent iron (nZVI) particles. They were synthesized by the borohydride reduction method, and then examined for reduction of perchlorate in various concentrations, PH, temp and additional technics. To improve the efficiency of reduction of perchlorate, we used stabilizer such as alginate, starch or SDS surfactant. We also investigated how the stabilized nZVI particles influence their reactivity toward perchlorate. In this study, the effect of stabilizer on reductive perchlorate was also investigated using nZVI particles.

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An Aggregation-Based Immunoassay using Surface Enhanced Raman Scattering

정은수, 주재범

한양대 바이오나노공학과

Immunoassay always plays an important role in clinical diagnostics and biochemical studies. Recently, antibody-coated nanoparticles are extensively used for fast and sensitive immuno-analysis. The reaction of the antibody-coated nanoparticles with the corresponding antigens resulted in the cross-linking of the particles that led to their aggregation. This aggregation property quantitatively changes with respect to the amount of the antigen. Thus, aggregation degrees can be used for a quantitative analysis of a specific antigen. The aggregation-based immunoassay has some advantages that nanoparticles form more stable suspensions and less susceptible to nonspecific aggregation. Since the aggregation of gold nanoparticles causes an absorption change, the rate of aggregation of gold nanoparticles can be determined by measuring the absorption change of the gold colloid suspension. On the other hand, the SERS peak change, caused by the density variation of 'hot spots', is known to be much more sensitive than the variation of broad UV/Vis absorption band. In the present study, thus, a SERS detection was utilized for quantitative analysis of a specific antigen.

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The development of simultaneous determination method for corticosteroids

박수민, *염혜영, 팽기정

*연세대 화학과 *서울의료원 아토피 클리닉*

Atopic dermatitis, one of the atopic diseases, is chronic recurrent diseases developing symptoms of pruritus and distinguishing skin types. Although the cause and occurrence route are not yet known, various causes maybe participated in atopic dermatitis. A part external steroid application consisted of corticosteroid hormone and humectants are used to treat atopic dermatitis. Corticosteroid has strong anti-inflammatory effect, so that is essential for treatment of atopic dermatitis. However, sometimes corticosteroid can lead to dermatitis and aggravate diseases, so additional cure is required to avoid side effects. Corticosteroid is divided into seven groups by the potency. Our objective substances are clobetasol propionate, betamethasone dipropionate and fluticasone propionate in high potency groups. Recently, betamethasone derivative is detected in cosmetic product which doesn't represent its ingredient. In many cases, companies do not show the containing percentages of corticosteroids in cosmetic product. Therefore, we studied a simultaneous analysis method of corticosteroids by liquid chromatography - tandem mass spectrometry and applied to humectants. In this study, in order to effectively extract clobetasol propionate, betamethasone dipropionate and fluticasone propionate from humectants came into the market, solid phase extraction is utilized and the analytical process for aforementioned corticosteroids is optimized.

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Highly sensitive trace analysis of paraquat using a surface-enhanced Raman scattering microdroplet sensor

Rongke Gao, *최남현, **장수익, *주재범

*한양대 응용화학과 *한양대 바이오나노공학과 **충북대 생화학과*

We report a rapid and highly sensitive trace analysis of paraquat (PQ) in water using a surface-enhanced Raman scattering (SERS)-based microdroplet sensor. Paraquat is a highly effective contact herbicide that is worldwidely marketed as a fast-acting, non-selective compound for broadleaf weed control. Compared with most pesticides, however, PQ is extremely toxic to humans and the lack of strategies to manage PQ poisoning has resulted in high fatality rates. Aqueous samples of PQ, silver nanoparticles, and NaCl as the aggregation agent were introduced into a microfluidic channel and were encapsulated by a continuous oil phase to form a microdroplet. PQ molecules were adsorbed onto particle surfaces in isolated droplets by passing through the winding part of the channel. Memory effects, caused by the precipitation of nanoparticle aggregates on channel walls, were removed because the aqueous droplets were completely isolated by a continuous oil phase. The limit of detection (LOD) of PQ in water, determined by the SERS-based microdroplet sensor, was estimated to be below 2×10-9M, and this low detection limit was enhanced by one to two orders of magnitude compared to conventional analytical methods.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Development of a Spectroflourimetric Method for the Determination of Dopamine by its Enhancement Effect on the Fluorescence of Terbium (III) Sensitized by Silver Nanoparticle

MD.KAMRUZZAMAN, *김소연, *조해진, *서연숙, *이상학

*경북대 화학과 분광분석 실험실 *경북대 화학과*

A new sensitive, simple and selective spectroflourimetric method was developed for the determination of biologically important compound dopamine in pharmaceutical formulations and biological fluids. This method is based on the sensitized fluorescence of terbium(III) when excited in the presence of dopamine (DA) because a Tb(III)–DA complex is formed and the maximum fluorescence peak locates at 545 nm. A pronounced enhancement of intensity at 545 nm was observed when the silver nanoparticles were added to the Tb(III)–DA system in the presence of an anionic surfactant, sodium dodecyl benzene sulphonate and the relative intensity is proportional to the concentration of DA. The different experimental parameters affecting the development and stability of the reaction product were carefully studied and optimized. At the optimized conditions, the present method allows the determination of dopamine in the linear range of 1.7×10^{-10}-7.6×10^{-8}mol L^{-1} with a correlation coefficient of 0.9999. The limit of detection (LOD) as defined by IUPAC (C_{LOD} =3×Sb/m, where Sb is the standard deviation of the blank signals and m is the slope of the calibration graph) was found to be 8.1×10^{-11}mol L^{-1} and the relative standard deviation (RSD) is 1.35% for 5 determinations of 2.5×10^{-8} mol L^{-1} dopamine. The proposed method showed good stability and reproducibility and applied satisfactorily to the determination of dopamine in pharmaceutical preparations and serum sample.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Removal of hexavalent chromium from aqueous solution by iron alginate

김진산, 강상혁, 팽기정

연세대 화학과

An interest for biosorption for water remediation has increased in recent years. In this study, we present an evaluation of hexavalent chromium removal in aqueous solutions using iron alginate. iron alginate was prepared from alginic acid extracted from fresh algae, edible seaweed(Undaria pinnatifida) which is a kind of brown seaweeds using tailored extraction method. We confirmed that iron alginate was made from an alginic acid with FT-IR spectra in the preliminary work. Cr(VI) is one of the major pollutant of groundwater and could be fatal in human body with a few ppm level. Stabilized iron alginate net can be an important adsorbent of Cr(VI) for rehabilitation of contaminated water. The process is pH dependent, we found the optimum pH range under various ascorbic acid condition. From a 300 mg/L to 0.05 mg/L, more than 95% of Cr(VI) was removed. Iron alginate is good choice for the remediation of heavy metals in surface water.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Development of carbon linked substituted polyaniline as a new support matrix for nickel based catalysts

이광필, *A.Gopalan, *Shanmuga sundaram Komathi, **이세희, ***M. Francklin Philips, ****김경웅

*경북대 화학교육과 *경북대 화학과 **경북대 나노과학기술과 ***경북대 차세대에너지기술연구소 ****경북대 나노과학기술과, 주식회사 크레진 연구소*

Recently preparation of porous conducting polymer networks is attracting specific attention for the immobilization of biomolecules and as support for loading of electrocatalysts. Herein, a new carbon coupled porous substituted polyaniline network (C-SPANI(NW)) was prepared by one-step polymerization of substituted aniline in the presence of carbon and a cross linking agent using ammonium persulfate as oxidant. Then transition metal ions of Ni(II) were incorporated to the C-SPANI(NW) by cyclic voltammetry. The electrochemical characteristics of the Ni deposited (C-SPANI(NW)) nanocomposite (designated as C-SPANI(NW)/Ni-NC) was investigated in 0.1M NaOH solution. The morphology and microstructure of the C-SPANI(NW)/Ni-NC were evaluated by field emission scanning electron microscope, X-ray diffraction (XRD) and X-ray photoelectron spectroscopy. C-SPANI(NW)/Ni-NC was investigated for its electrocatalytic activity towards the oxidation of methanol. The influences of support matrix (C-SPANI(NW)) in the distribution of Ni(II) and its electrocatalytic activities were explored.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Preparation of a new hole transport material based on carbon nanostructures dispersed into substituted polyaniline for solar cell application

이광필, [*]Kruthiga Gopalan, [*]Krupa Gopalan, [**]Shanmuga sundaram Komathi, [***]이세희, [**]A.Gopalan, [****]김경웅

경북대 화학교육과 [*]Rajalakshmi Engineering College, Thandalam, Chennai, India [**]경북대 화학과 [***]경북대 나노과학기술과 [****]경북대 나노과학기술학과, 주식회사 크레진 연구소

Solar cells will be one of the main alternative-energy sources in the near future. Polymer solar cells (PSC) are promising because they would be much cheaper to produce and far more lightweight than conventional solar cells. Currently the efficiency of PSC is around two percent. Recently, the utilization of thin films of carbon based nanostructures as the hole transport and electron blocking layer in PSC attracts research interest. In this work, we report the preparation of a new hole transport material by chemical polymerization of substituted aniline (SPANI) in the presence of cross linker and carbon nanostructures (C(NS)) using ammonium persulfate as oxidizing agent. The chemically prepared C(NS)/SPANI nanocomposite (designated as C(NS)/SPANI-NC) has been evaluated for morphology by field emission scanning electron microscopy. The optical transparency of C(NS)/SPANI-NC thin film was analyzed by UV-visible spectroscopy. A miniaturized PSC was constructed using C(NS)/SPANI-NC as hole transport layer. The solar cell characteristics such as the current-voltage plots and open-circuit voltage (Voc) of the devices were determined. The performance influences on film thickness and the amount of C(NS) were analysed.

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Application of Flow Injection Cold Vapor Isotope Dilution Inductively Coupled Plasma Mass Spectrometry in Marine Sediment and Fly Ash for the determination of Mercury

MD.KAMRUZZAMAN, *이상학

*경북대 화학과 분광분석 실험실 *경북대 화학과*

In this work, Flow Injection-Isotope Dilution-Cold Vapor -Inductively Coupled Plasma Mass Spectrometry (FI-ID-CV-ICP/MS) was applied to determine trace level of mercury in fly ash and marine sediment. ^{202}Hg isotopic spike was added to 0.25 g of BCR176R fly ash and 0.1 g of NIST 2702 marine sediment sample and then was decomposed by microwave digestion procedure with acid mixture A (8mL HNO_3+2mL HCl+2mL HF) and acid mixture B (8mL HNO_3+2mL $HClO_4$+2mL HF) for applying IDMS. Mercury cold vapor was generated by using reductant solution of 0.2 %(w/w) $NaBH_4$/0.05%(w/w) NaOH. The measurements of ^{200}Hg (spike)/^{202}Hg (reference) isotope ratio was made using a quadrupole ICP/MS system. The accuracy of this method was verified by the analysis of certified reference material (CRM) of fly ash (BCR 176R) and sediment (NIST 2702). The indicative value of Hg in BCR 176R fly ash was 1.60±0.23 mg/kg (k=2), and the certified value of Hg in the NIST 2702 sediment CRM was 0.438±0.024 mg/kg (k=2). The determined values of Hg in BCR 176R fly ash and NIST 2702 sediment CRM by the method of FI-CV-ID-ICP/MS described in this paper were 1.60±0.24 mg/kg (k=3.18) and 0.454±0.05 mg/kg (k=3.18) respectively, and these results agree well with certified or indicative value within the range of uncertainty.

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A simple one pot synthesis of a new conducting polymer based nanomesh

A.Gopalan, Shanmuga sundaram Komathi, *이광필

*경북대 화학과 *경북대 화학교육과*

A one pot synthesis has been developed for the preparation of a new support matrix, functionalized carbon (FC) interlinked polymeric nanomesh (NM), towards using in biosensors. FC was chemically interlinked to substitiuted polyaniline (SPANI) and the NM was formed through enzyme (Horse raddish peroxidase (HRP)) catalyzed polymerization of aniline in the presence of a cross linker and a mesh forming additive. The resulted FC interlinked substituted polyaniline NM with insitu entrapped HRP is designated as FC-SPANI(NM)/HRP. For the comparison, the enzyme-free FC-SPANI(NM was also preparaed using ammonium persulfate as the oxidizing agent. Also, simple SPANI(NM), in the absence of FC support, was prepared. The morphology of prepared NMs was examined by field emission scanning electron microscopy. The electronic states and the structural aspects of the PANI(NM) and the insitu entrapped HRP were investigated by UV-visible spectroscopy, Fourier transform IR spectroscopy. The utility of FC-SPANI(NM)/HRP was evaluated as an electrochemical biocatalyst for the development of third generation hydrogen peroxide (H_2O_2) sensor.

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Preparation of palladium particles dispersed poly(diphenylamine-co-3-aminobenzonitrile) composite and evaluation as electrocatalyst

M. Francklin Philips, *A.Gopalan, **이광필

*경북대 차세대에너지기술연구소 *경북대 화학과 **경북대 화학교육과*

A new supporting matrix, poly(diphenylamine-co-3-aminobenzonitrile) (P(DPA-co-3ABN), has been exploited to disperse palladium particles (PdNPs) for the preparation of P(DPA-co-3ABN)-Pd catalyst. The prepared P(DPA-co-3ABN)-Pd catalyst has been characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD) analysis. The electrocatalytic activity of the P(DPA-co-3ABN)-Pd catalyst towards oxidation of formic acid has been examined in acidic solution by cyclic voltammetry and chronoampermetry. The results indicate enhanced electrocatalytic activity towards formic acid oxidation for P(DPA-co-3ABN)-Pd catalyst as compared with PDPA-Pd catalyst. The enhanced electrocatalytic activity of P(DPA-co-3ABN)-Pd catalyst is due to incorporation of 3ABN units into the PDPA matrix which stablize PdNPs as well as resist the leaching out of PdNPs from the substrate.

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Sensitive Chemiluminescence Determination of Enoxacin by Flow–injection Analysis in Biological Fluids and Pharmaceutical Formulation Using Copper (II) in Luminol-H_2O_2 System

ALAM MD AL MAHMNUR, *이상학, **김영호, *정혜영, *서연숙

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A sensitive chemiluminescence (CL) detection method by flow injection analysis (FIA) was investigated for the assay of enoxacin (ENX) using luminol-H_2O_2 system in presence of copper (II). It was observed that interaction of ENX with copper (II) caused the sensitization of CL intensity of the system strongly. Based on this, a rapid and sensitive CL-FIA method was designed for the determination of trace amount of ENX. Under optimum experimental conditions, the enhancement of CL was linear with the concentration of ENX in the range of $5.5\times10^{-10}$to 3.0×10^{-7} molL^{-1} (r=0.9998) with a detection limit, as defined by IUPAC, $C_{LOD} = 3\times S_b/m$ (where S_b is the standard deviation of the blank signals and m is the slope of the calibration curve) of 3.5×10^{-10}molL^{-1}. Precision of the method was tested at the concentration level of 1.0×10^{-7} molL^{-1}for 11 replicate measurements giving value of relative standard deviation (RSD) 1.25%. The proposed method was successfully applied for quantitative determination of enoxacin in biological fluids (human serum and urine) and pharmaceutical formulation.

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Preparation of new catalyst based on carbon nanotubes supported gold nanoparticles for direct methanol fuel cells

이세희, *M. Francklin Philips, **A.Gopalan, ***이광필, ****김경웅

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Gold nanoparticles were anchored onto thiol functionalized multi walled carbon nanotubes using a stabilizing linker (SL) and supported catalysts (AuNPs-SL-MWNT-SH) have been successfully prepared. The morphology and microstructure of NPs-SL-MWNT-SH were examined by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) analyses. The electrocatalytic activity of the AuNPs-SL-MWNT-SH catalyst was examined towards oxidation of methanol by cyclic voltammetry for various concentrations of methanol in 0.5M H2SO4. The membrane electrode assembly (MEA) was fabricated using Nafion 117 as the membrane by loading AuNPs-SL/MWNT-SH as anode catalyst and conventional cathode materials. The simple preparation method and excellent performance of the NCNT-based Au catalysts indicate their potential application in direct methanol fuel cells.

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Investigation of the structure, swelling and drug release characteristics of poly(N - isopropyl acrylamide) based composite hydrogels

김민경, **A.Gopalan,** *이광필

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Gels that set from liquid to solid under physiological conditions are of particular interest as biomaterials due to their recognized usefulness for drug delivery. Polymers that gel in response to changes in physiologically relevant stimuli, such as pH, ionic strength or temperature, are appealing in biomedical applications due to their benign setting process. Their gelation process is free of toxic synthesis reagents or harsh chemical reactions, which preserves the viability of entrapped cells or biomacromolecules or drugs. Medical and biological uses of thermoresponsive polymers require control over their mechanical properties and swelling. The thermomechanical characteristics of these systems are critical to their clinical handling characteristics, resistance to physiological stresses and the response of native or implanted cells , while swelling dictates their water content and dimensional stability. Even amongst hydrogels and many copolymers of N-isopropyl acrylamide (NIPAAm)] based thermoresponsive polymer systems, diverse variation in gelation characteristics exist, including critical concentrations, gelation rates, volume changes and mechanical properties. In this work, Microgels based on NIPAAm, were prepared by Ultra violet radiation initiated free radical polymerization method. The behavior of these microgels was studied with respect to their swelling, and release properties. Water uptake was tested for the gels containing different amount of NiPAAm monomer. This study provides the background for the design of an injectable device suitable for the controlled delivery of the drug.

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Spectrofluorimetric Study of Nanosilver Sensitized Luminescence of Terbium (III) For the Determination of a Catecholamine in Human Serum and Urine

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In the present study, a new spectrofluorometric method was developed for the determination of epinephrine based on the nano-silver sensitized fluorescence of Terbium (III)-Sodium Dodecyl Benzene Sulfonate (SDBS)-Epinephrine (EPN) system. Terbium (III) ion can form strong complex with Epinephrine in basic medium (pH 9.0) in presence of sodium dodecyl benzene sulfonate. Intramolecular energy transfer takes place when the system is excited at 290 nm and the enhancement of fluorescence intensity was found maximum at 545 nm which is the characteristic fluorescence of Terbium (III). When the colloidal suspension of silver nano particle was introduced into Tb (III)-SDBS-EPN system, the luminescence intensity at 545 nm was greatly increased. Under the optimum experimental conditions, relative enhancement of fluorescence intensity was linear with the concentration of EPN in the range of $3.1\times10^{-10}$to 3.5×10^{-8} mol L^{-1} (r=0.9997) with a detection limit of 2.48×10^{-10}mol L^{-1}. The Relative Standard Deviation for 10 repeated measurements of 1.0×10^{-8} mol L^{-1} EPN was 1.27%.The proposed method was successfully applied for quantitative determination of epinephrine in human serum and urine.

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Synthesis and characterization of bi-component conducting polymer nanostructures containing carbon fillers for electronic application

Shanmuga sundaram Komathi, *Krupa Gopalan, *Kruthiga Gopalan, **이세희, A.Gopalan, ***이광필

*경북대 화학과 *Rajalakshmi Engineering College, Thandalam, Chennai, India **경북대 나노과학기술과 ***경북대 화학교육과*

Conductive polymer nanostructure composites (CPNSCs) have attracted much attention over the last few years due to their application in flexible electronics, electromagnetic shielding, electrostatic dissipation and as PTC elements for self regulated heating applications and switching devices. Most of applications for electronic devices employing composite films required adhesion to a substrate within a particular microelectronic circuitary where the difference between properties of the composite film and the substrate may influence the physical behaviour of the composite film. A new concept is described that creates multifunctional conducting polymer nanocomposite tapes that combine electrical and nanoscale properties of a conductive polymer and a low percolation threshold of conductive nanofillers. The concept is based on a bicomponent construction consisting of conductive polymer layer as core and carbon filler as shell. Herein, we report the preparation of the new carbon loaded CPNSCs using polymerization coupled with loading of carbon fillers in a singe step. The morphology and microstructure of CPNSCs was evaluated using scanning electron microscopy and X-ray diffraction analysis. The electronic properties of CPNSCs were obtained through UV-Visible spectroscopy. The current-potential characteristics of the CPNSCs films were evaluated. The interfacial characteristics of the CPNSCs were investigated by electrochemical impedance spectroscopy.

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Electrochemical deposition of conducting polymer and gold nanoparticles multi-layer films

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A simple route to the fabrication of multilayer films containing conducting polymer (CP) and gold nanoparticles (AuNPs) is described. Multilayer films of CP and AuNPs were grown in a systematic and controlled manner on Indium Tin Oxide coated glass plate. For the multilayer electrodeposition, potentiostatic pulses were applied by choosing proper experimental conditions such as pulse number, pulse width, lower and upper potential limits and cathodic and anodic pulse durations. Electrochemical characteristics of the film electrodes having alternative layers of electrodeposited CP and AuNPs have been evaluated by cyclic voltammetry. The physic0-chemical properties of the films were characterized by XRD, XPS, SEM, TEM and AFM analysis.

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Nanocrystalline carbon –polynailine composite : preparation and prospective use in portable glucose biosensors

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A new nanocomposite based on nanocrystalline carbon (NCC) and polynailine (PANI) has been successfully prepared by electrochemical grafting of PAN) chains onto NCC surface (NCC-g-PANI). The morphology of NCC-g-PANI was examined by field emission scanning electron microscopy. The structural and the electronic states of PANI were investigated through UV-visible and fourier transform IR spectroscopy. The electrochemical behavior and the interfacial characteristics of the fabricated NCC-g-PANI were investigated by cyclic voltammetry and impedance measurements. The NCC-g-PANI- NC provides ideal biocompatible environment for loading enzymes. We anticipate that NCC-g-PANI- NC matrix can have the ideal characteristics for the fabrication of portable biosensors.

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A Sensitive APUTP Method for Measuring Bulk Nickel and Copper in Silicon Wafer

이성욱, 이상학, *김영호, **ALAM MD AL MAHMNUR

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The new metrology for measuring bulk Cu and Ni in heavily boron doped wafer was developed, that is called APUTP. The Ni recovery rate of 98.8% and Cu recovery rate of 96% were achieved through optimizing the vapor phase etching and the condition of wafer surface scanning after the poly-silicon layer Cu and Ni was captured was etched with acid vapor phase. The lower method detection limit could be achieved through automating each unit processes that had been done manually in traditional PUTP method. This advanced PUTP method could give a good explanation for contamination paths of Cu, Ni to silicon wafers during wafer manufacturing. It was found that the higher amount of bulk Ni contamination arose during etching with KOH in heavily boron doped silicon compared with lightly boron doped wafer, and bulk Cu contamination was introduced when polishing with slurry including amine.

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A Sensitive Flow-Injection Chemiluminescence Determination of Norfloxacin Based on its Enhancing Effect on the Luminol-H_2O_2 System Catalysed by Copper

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*경북대 화학과 *경북대 화학과 분광분석연구실*

A rapid and sensitive flow-injection chemiluminescence method is proposed for the determination of norfloxacin (NFLX) in pharmaceutical preparations and biological sample. The method is based on the fact that the weak CL from the reaction of luminol-H_2O_2 can be greatly strengthened by Cu(II). Thus, on injection of NFLX into the luminol-H_2O_2-Cu (II) system, the CL intensity is substantially increased. The enhancement effect is attributed to a catalytic effect of Cu (II) due to the interaction caused by NFLX which forms a complex with the catalyst. The experimental parameters were optimized systematically. Under the optimal conditions, the sensitizing effect of the CL intensity is proportional to the concentration of NFLX in the range of 8.9×10^{-10}-4.0×10^{-7} mol L^{-1} (r=0.9999) with a detection limit (3σ) of 2.08×10^{-10} mol L^{-1}. The proposed method had good reproducibility with the relative standard deviation (RSD, n=7) of 1.19 % for 2.6×10^{-7}mol L^{-1} of NFLX. The possible reaction mechanism of the CL reaction is also discussed. This method has been successfully applied for the determination of trace amount of NFLX in pharmaceutical preparations and serum samples.

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A Chemiluminescence Method for the Determination of Copper Ion (II) Using Phosphate Buffer

조해진, *MD.KAMRUZZAMAN, 이상학, **김영호

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Determination of copper ion (Ⅱ) in aqueous solution by chemiluminescence (CL) method using a batch type system has been studied. The effect of copper ion (Ⅱ) concentration on the CL intensity in the oxidation reaction of luminol with hydrogen peroxide was applied to the determination of copper ion (Ⅱ). The effects of pH, concentration of luminol and hydrogen peroxide and phosphate buffer on the CL intensity were investigated. The CL intensity of luminol was further increased with addition of phosphate. The calibration curve for copper ion (Ⅱ) was linear over the range from 5.5×10^{-10} to 6.5×10^{-8}mol L^{-1} and detection limit was 4.0×10^{-11}mol L^{-1} under the optimal experimental conditions of 2.5×10^{-2}M, 0.1M, 13.0 for concentration of hydrogen peroxide, phosphate buffer, and pH, respectively.

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Analysis of creatinine in human serum by isotope dilution liquid chromatography-tandem mass spectrometry

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Creatinine in serum was measured for the providing of reference value of a proficiency testing. The reference values were determined by isotope dilution liquid chromatography tandem mass spectrometry accepted as a candidate reference method. Because IDMS has advantages such as a providing of uncertainty, correction of recovery and the elimination of matrix interferences, it is recognized as a candidate reference method. Isotopically labeled internal standard was creatinine-d3. The LC/MS/MS used in this study was a triple-stage quadrupole mass spectrometer, model API 4000 MS/MS, combined with an Agilent 1200 HPLC through its electrospray ionization interface. Creatinine was monitored by summation peak of mass transfer m/z 114.1/44.1 and 114.1/86.1 and creatinine-d3 by summation peak of mass transfer m/z 117.1/47.1 and 117.1/89.1. The used column was a Thermo Hypersil GOLD C18 (50 x 2.1 mm, 3 μm). The mobile phase was 10 mM ammonium acetate and flow rate was 0.2 mL/min. The injection volume was 5 μL. The serum samples were four kinds of KRISS CRMs and three kinds of the proficiency testing materials. Method validation was proved by participating in CCQM key comparison. And the result showed equivalence with reference value within uncertainty.

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Raman vibrational studies of the mycotoxin Zearalenone and its derivatives by Raman spectroscopy

강원석, 김효섭, **Najeeb.C.K**, 연찬미, 안대희, 김재호

아주대 분자과학기술학과

Zearalenone (ZEN) is a mycotoxin produced by several species of the genus Fusarium, mainly Fusarium graminearum. This mycotoxin and its derivatives (Zearalanone(ZAN), Zearalenol(ZENOL), Zearalanol(ZANOL)) are frequent contaminant of cereal crops, such as maize, barley, oats, wheat and other grains throughout the world. For this reason, many countries of the world have established maximum tolerance range of these mycotoxin from 30 to 1000 μg/kg in grains. In this study, Raman spectroscopic technique which is well known as a non-destructive analytical tool for the in situ identification of both organic and inorganic materials, was used to characterize the ZEN and its derivatives. Raman spectra were collected using a triple monochromator coupled with a CCD array detector (Triplemate 1877, Spex Industries, Edison, NJ, USA). And laser power for all experiments was used 15 mW at 514.5 nm (Innova 70 Ar+ laser, Coherent Co., CA., USA). The C=C stretching vibrational modes of ZEN and ZENOL appeared at 975-990 cm-1. The C=O vibration mode showed at 1680-1690 cm-1 for ZEN and ZAN, but didn't showed in ZANOL and ZENOL which have –OH group instead of -C=O group in ZEN and ZAN molecular structures. On the basis of this characterization, Raman spectra of specific chemical groups and linkages corresponding to the structural difference of ZEN and its derivatives were identified. These results indicated that Raman can apply for the identification of ZEN and its derivatives and has a potential for the non-destructive rapid detection of ZEN and its derivatives in food. In our future work, we will study the Raman spectroscopy of mixed sample with corn and wheat for the non-destructive rapid detection of mycotoxin.

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Comparison of MALDI TOF-MS and HPLC quantification methods for N-acetylglucosamine

홍장미, 신성재, 양효직, 김진희, 이선영, 박세환, 김정권

충남대 화학과

Quantitative information for N-acetylglucosamine (GlcNAc) was obtained using High-performance liquid chromatography (HPLC) with Ultraviolet (UV) and refractive index (RI) detectors and Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS). RI detection is commonly used in the analysis of molecules which do not have an absorption in the UV range. In the current analysis of GlcNAc, GlcNAc shows a strong absorption at 194nm. While the sensitivity using UV was much better than that uing RI, RI provided better linearity. MALDI-MS is a simple and rapid technique with high accuracy. Since MALDI analysis is known to have very poor reproducibility, and an internal standard will be used. In conclusion, the quantitative analysis of GlcNAc is performed using three different techniques; HPLC-UV, HPLC-RI and MALDI-MS.

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Preparation of polystyrene on initiator attached silica monolith particles by radical polymerization for a new type stationary phase in HPLC

이승미, 정원조

인하대 화학과

There have been extensive studies in controlled polymerization of organic monomers on porous or nonporous inorganic surface by making use of a surface attached initiator. The resultant organic-inorganic combined polymer can be used as stationary phases in chromatography. In this study, initiator bonded monolith silica particles have been prepared and used to make a new stationary phase by reversible addition-fragmentation chain transfer (RAFT) polymerization. Silica monolith particles were obtained from the polymerization product prepared by heating the reaction mixture of tetramethylorthosilicate (TMOS), polyethylene glycol(PEG), and acetic acid. The monolith silica particles were reacted with (3-choloropropyl) trimethoxysilane followed by sodium diethyldithiocarbarmate to make initiator attached silica monolith particles. The dried initiator monolith particles were then allowed to undergo radical polymerization with styrene to give a new stationary phase. We investigated separation performance of the prepared stationary phases in HPLC. The new stationary phase was packed in a glass-lined stainless steel microcolumn (300×0.5mm) to examine its separation performance. The results were satisfactory. We were able to attain the numbers of theoretical plates up to 30.000.

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Sensitivity enhancement of Ag/Au Nano-structured SPR Chip by optimization of the deposited Au thickness

연찬미, 김효섭, 강원석, **Najeeb.C.K**, 김재호

아주대 분자과학기술학과

The surface plasmon resonance (SPR) has been widely employed for biosensor applications because of the capability for label-free detection of biomolecular interactions. However, the sensitivity of SPR sensor is lower than the conventional labeling immuno-sensing methods. The metal nanostructure-amplified surface plasmon resonance (SPR) analysis has been numerically investigated to enhance the sensitivity. In this study, we used trigonal pyramid shaped Ag nano-structures coated with 50 nm-Au-thin-film for SPR sensitivity enhancement.We used the Langmuir-Blodgett (LB) method for the preparation of large area, monolayer silica particle film as a template for fabricating the nano-structure Ag pattern on the flat 18x18 mm2 cover glass substrates. Ag nanostructures were formed by sputtering Ag film on the 300 nm silica nanoparticle LB layer on the glass substrates. After that, the silica LB layer was removed by sonicating. Upper Au thin-film was deposited by sputtering method in four deferent thicknesses. The thicknesses were 26, 43, 49, 62 nm and these figures were caculated by measuring bare SPR signals and math fitting.The sensitivity amplification of Ag/Au nano-structured SPR chip was evaluated by measuring the SPR angle shift between water and 20 % aqueous ethanol solution compared with conventional flat Au chips. The Ag/Au nano-structured SPR demonstrated a sensitivity enhancement up to 150 % compared to a conventional SPR chip.

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A research on the analytical method to determine total arsenic and arsenic species in seaweeds

나진수, **CUI SHENG**, 김유나, 남상호

목포대 화학과

The quantitation of the total arsenic in seaweed has routinely been performed. But, it has been very well known that toxicity and biological effect depend not only on the total concentration of As but also on the chemical species of As in sample. Of the chemical species of As, As^{3+} and As^{5+} are highly toxic. Therefore, the importance on research of arsenic speciation has greatly increased. It is necessary to develop the analytical method of As species because oxidation states of arsenic species should not be converted into each other during sample preparation. In this study, we have focused on the analytical method of total arsenic by ICP-OES (Inductively Coupled Plasma - Optical Emission Spectrometer) and the speciation method of arsenic species (As^{3+}, As^{5+}, MMA and DMA) using ICP-OES coupled with IC (Ion Chromatography) in several seaweeds (laver, green laver, sea tangle and sea mustard). The 10 % HNO_3 was used for extraction of total As, and mixture of methanol and water (1:1) was used for extraction of As species.

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Development of high-performance liquid chromatographic method for quantification of glucosamine

이선영, 김진희, 신성재, 양효직, 홍장미, 박세환, 김정권

충남대 화학과

Glucosamine (GlcN), an essential amino-monosaccharide reagent, is commonly found in connective tissues and gastrointestinal mucosal membrane. Analysis of glucosamine using typical reversed-phase column is difficult because of its early elution time. In this study, the chromatographic separation is achieved using an amine column. Quantitative information for GlcN is obtained using High-performance liquid chromatography with ultraviolet (UV) at a wavelength of 191 nm, refractive index (RI) and tandem mass spectrometry (MS/MS) (parent ion of m/z 180.1 and daughter ions of m/z 72 and m/z 162). Isocratic elution is used with a mobile phase of ACN:H_2O (75:25) at a flow rate of 1 mL/min.

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GPC characterization of N-allylated Poly(p-phenylene terephthalamide)

권혁주, 김건성, 이귤섭

효성기술원 분석센터

Poly(p-phenylene terephthalamide) (PPDT) is a rigid polymer having strong hydrogen bonding between amide proton and carbonyl group. Due to strong intermolecular interactions, their solubility in common organic solvents is extremely poor and this drawback does not allow PPDT molecular characterization. In this work, allyl group has been introduced to PPDT and its solubility in organic solvent such as $CHCl_3$ is dramatically enhanced. ^{1}H-NMR spectra of N-allylated PPDT (NA-PPDT) has shown that NA-PPDT has been successfully obtained and relative molar mass data of N-allylated PPDT has been obtained by SEC and compared with its intrinsic viscosity.

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Probing Heterogeneous Reaction Dynamics and Kinetics of Cholesterol and Unsaturated Phospholipid in Surfactant Lipid Layers Using Spectroscopic Techniques

고재윤, 허성우, 김성남, 김준곤, 김승빈

포항공과대 화학과

We present the study of heterogeneous oxidation of mixed lipid layers on the surface of sodium chloride particles. Monolayer-equivalent amounts of mixtures of phospholipids and cholesterol are prepared on the surface of sodium chloride particles. Heterogeneous reaction dynamics and kinetics of cholesterol and 1-palmitoyl-2-oleoyl-phosphatidylglycerol (POPG) and ozone at the air-solid interface have been studied using diffuse reflection infrared Fourier transform spectroscopy (DRIFTS). Distinct reaction dynamics and kinetics are observed from the heterogeneous reactions of cholesterol and POPG in the mixed lipid layers with ozone. Compared to the reaction rates of the ozonolysis of cholesterol and POPG alone, lower reaction rates of ozonolysis are observed when these lipids are present with unreactive saturated phospholipid, 1,2-dipalmitoylphosphatidylglycerol (DPPG). The relative medial location of unsaturated carbons of cholesterol and POPG is also investigated via competitive heterogeneous oxidation by ozone.

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APPLICATION OF THE JUDD – OFELT THEORY TO THE $Dy3^+$ DOPED FLUOROBORATE GLASSES

buithehuy

창원대 화학과

The optical characterizations of $Dy3^+$ doped in a series of glass samples $NaF-B_2O_3-Al_2O_3$ and $CaF_2-B_2O_3-Al_2O_3-CaSO_4$, synthesized by the fusion method, have been studied by Judd - Ofelt theory. The density, the refractive index, the optical absorption, the Judd-Ofelt parameters Ω2, branching ratios and the transition probabilities have been determined. Effects of Na, Ca and sulphate on the photoluminescent intensity, life time and luminescent yield have been explained.

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Simultaneous determination for antibiotics by dispersive solid-phase extraction and liquid chromatography-tandem mass spetrometry

이경준, 김소연, 이계호

충남대 화학과

가축의 생산성 및 질의 향상을 증가시키기 위한 목적으로 동물의약품이 과다 사용되어지고 있다. 이는 가축뿐만 아니라 최종 소비자인 인간에게도 생리학적인 장애 또는 내성이 생기는 문제를 야기 시킬 수 있다. 이러한 문제가 발생하는 것을 예방하기 위해 EU 에서는 최대잔류허용량을 규정하고 있으며, 더 효율적이고 정확한 결과를 얻기 위한 방법이 연구되고 있다. 이 실험에서는 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 시료 중 잔류하는 항생제 확인에 대하여 새로운 분석법을 확립하였다. 시료에 항생제 표준용액과 내부표준물질을 첨가하여 분석하였으며, 최적화된 전처리 방법과 기기조건을 찾아내었다. 본 실험을 통하여 최적화된 전처리 방법을 개발하고 최적의 기기 조건을 찾음으로써 여러 가지 시료와 분석 물질에 적용되어 유해 물질의 분석과 여러 분야에 쉽게 응용될 것이다.

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Investigation on the Electrochemical Behavior of Polyethylene glycol (PEG) Molecules in Trivalent Chromium Electrolytic Solution

Van Phuong NGUYEN

창원대

Polyethylene glycol (PEG), an organic additive, has been commonly used in various electroplating process, especially in copper, zinc and nickel plating industry. Generally, the main function of PEG molecules in the electroplating solution is to increase its current efficiency and enhance the surface characteristics of electrochemically deposited layer – surface evenness, hardness, brightness and corrosion resistance. Hence, the reactions of PEG molecules with trivalent chromium ions and their effectiveness to trivalent chromium plating process were investigated intensively. For this purpose, we used electrospray ionization mass spectrometry (ESI-MS), electrochemical quartz crystal microbalance (EQCM) technique, current efficiency measurements and scanning electron microscopy (SEM). It was revealed that the PEG molecules were stable in a trivalent chromium bath containing potassium formate. During electroplating process, the PEG molecules made the reductive current of trivalent chromium ions lower than PEG-free solution and promote a hydrogen evolution reaction through their adsorption and desorption on the cathode surface. The degradation of PEG molecules during electroplating process is under investigation.

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Solid-state ^{13}C NMR study of some typical forest soil samples

오세웅

목포대 화학과

Solid-state NMR spectroscopy on ^{13}C is a powerful tool to study forest soil. CPMAS-NMR techniques are assumed to be only semi-quantitative in the assessment of carbon distribution in natural organic matter. CP and NQS (non-quaternary suppression) ^{13}C spectra of some typical forest soil samples are presented with their IR spectra, SEM images and TOC data in this work. Also solid-state ^{13}C NMR spectra of some organic compounds of known structure related to the forest soil samples are shown.

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Qualitative and Quantitative Analysis of Flavonoids by Ultra Performance Liquid Chromatography couple with Quadrupole Time-of-Flight Mass Spectrometry using kinetic method

진광재

창원대 화학과

A novel method was developed to quantitative determination of diastereoisomeric pairs of flavonoids based on a fixed(nondissociating) ligand version of the kinetic method using ultra-performance liquid chromatography-quadrupole time-of-flight mass spectrometry detection(UPLC-QToF-MS). The flavonoids separation was carried out on an Acquity UPLC BEH C_{18} column with 0.2% formic acid and methanol as the mobile phase under gradient conditions. After the chromatographic separation, a pre-mixed solution containing an appropriate transition metal ion, a fixed ligand and a reference ligand was added to the target analyte by post-column to generate the singly charged transition metal ion-bounded clusters by electrospray ionization in the gas phase. The selective cluster ion was mass-selected and the kinetics of its competitive unimolecular dissociations was investigated in a quadrupole time-of-flight mass spectrometer under MS2 mode. Their characteristic mass spectrometric fragmentation patterns were studied and the corresponding fragmentation pathways were proposed. Quantitative determination of the isomeric compositions of the flavonoids were achieved by using constructed calibration curves.

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DSPE followed by gas chromatography mass spectrometry for the 125 multi-residue analysis of pesticides in agriculture

이동욱, 권종은, 이계호

충남대 화학과

전 세계적으로 농산물의 생산성 및 질의 향상을 증가시키기 위한 목적으로 농약이 과다 사용되어지고 있다. 하지만 이는 최종 소비자인 인간에게도 생리학적인 장애 또는 내성이 생기는 문제를 야기 시키기 때문에 현재 세계 각국에서 농약에 대한 MRL(Maximum Residue Levels)을 지정하여 규제를 하고 있다. 이 실험에서는 acetonitrile 을 이용하여 추출을 하였고, PSA 를 사용한 Dispersive-SPE 방법을 사용하여 경제적이고, 빠르며 많은 시료에 대해 쉽게 전처리를 할 수 있었다. 또한 GC-MS 를 이용하여 기존의 분석법보다 더 빠른 분석법에 대하여 연구하였다. Matrix matching calibration 을 하여 matrix 에 대한 효과를 최대한 줄였다. 또한 최적화된 전처리 방법과 기기조건을 찾아내었으며, 회수율 및 검정곡선의 재현성, 회수율에서 만족할 만한 결과를 얻을 수 있었다. 본 실험을 통하여 최적화된 전처리 방법을 개발하여 여러 가지 시료와 분석 물질에 적용하였다. 또한 동시에 다성분을 짧은 시간에 분석하는 조건을 확립하게 되었다.

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Trace analysis of mycotoxin in wine using dispersive solid-phase extraction followed by LC-MS/MS

권종은, 이동욱, 이계호

충남대 화학과

곰팡이 독소는 유해 곰팡이에 의해서 생성되는 2 차 대산물질로서 인간과 동물에 유해한 작용을 나타내는 유독물질을 총칭한다. 농산물의 생육기간 및 저장, 유통 중에 생성되며, 열에 안정하여 조리·가공 후에도 분해되지 않는다.

이에 오염된 식품이나 사료를 섭취한 사람이나 동물에게 여러 가지 장애를 일으키며 특히, 간암이나 식도암 등의 발암성과 관련이 있기 때문에 세계 각국에서 관심이 집중되고 있으며 식품안전성에 있어서 식품첨가물이나 잔류농약보다 곰팡이 독소의 위험이 더 큰 것으로 논의되고 있다. 또한 이 때문에 세계 각국에서 곰팡이 독소에 대한 MRL(Maximum Residue Levels)을 지정하여 규제를 하고 있다.

기존의 방법이나 공정법에는 Immunoaffinity column 을 이용한 전처리 방법을 이용하고 있으나, 이는 한 번에 한 물질에 대해서 분석을 하기 때문에 동시에 다성분을 분석하지 못할뿐만 아니라, 경제적인 이유 등으로 효과적이지 못한 면이 많다.

이에 따라 본 실험에서는 더욱 경제적이고, 다성분 분석을 동시에 하기 위해, 변형된 DSPE(Dispersive Solid Phase Extraction) 분석법을 개발하였고, 또한 LC-MS/MS 를 이용함으로써 여러 종류의 곰팡이 독소에 대하여 동시에 검출 할 수 있었다.

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Highly sensitive detection of mercury ions using aptamer-conjugated nanoparticles in nanoliter droplets

황선영, *이상엽, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과*

In this presentation, we report a conceptually new method for the trace analysis of mercury (II) ions in water. This involves the use of droplet-based microfluidics combined with SERS detection using aptamer-conjugated Au/Ag hybrid nanoparticles. This approach provides both fast and sensitive detection of mercury (II) ions in water. Here, the aptamer molecule used in this study is rich in thymine (T) and mercury (II) ions are effectively captured by readily forming T–Hg2+–T configuration. All the detection was proceeded in a microdroplet channel. Manipulation of such droplets through winding microchannels affords rapid and efficient mixing of the contents. Quantitative analysis of mercury (II) ions was performed by calculating spectral Raman peak area of Cy3 at 1,580cm−1. The proposed analytical method offers a rapid and reproducible trace detection capability for mercury (II) ions in water.

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Determination of a multi-residue for 54 pesticides in Brown Rice Green Tea by Liquid chromatography-tandem mass spectrometry and Dispersive Solid Phase Extraction

김소연, 이경준, 이계호

충남대 화학과

최근 세계적으로 건강에 대한 관심이 급증하고 있다. 이와 더불어, 우리가 과거에 식품의 질과 맛의 향상을 위해 사용되었던 화학 물질의 문제가 부각되어지자, 여러 국가 측면에서도 국민의 건강을 위해 이를 규제하고 연구를 진행하고 있다. 특히, 농산물의 농약사용과 관련하여 각국의 상황에 맞게, MRL(Maximum Residue Levels)을 규정하여 규제하고 있다.

Well-being 에 걸 맞춰서 아시아뿐만 아니라, 세계 곳곳에서 차 문화에 대한 관심도 또한 급증하였다. 우리나라에서도 많은 이들이 다양한 차를 즐기고 있는데, 이에 대한 재배과정에서의 약품처리에 대해서는 알고 있는 사실이 적다. 이처럼, 대중화된 차에 잠재적으로 함유되어 있는 농약에 대한 정확한 정보가 well-being 에 걸맞게 인식되어야 한다. 따라서, 이번 실험을 통해 alkaloids 나 polyphenol, pigments 등의 복잡한 matrix 를 갖고 있는 차 분석에 적합한 추출과정의 최적화와 다성분 농약의 동시분석을 가능하게 하는 분석방법의 최적화를 이용하여 잔류농약 분석 분야의 발전을 도모하고자 했다. 본 실험에서는 acetonitrile 을 이용하여 추출하였고, PSA, GCB 를 이용하는 Dispersive Solid Phase Extraction 방법을 사용하였다. 또한, liquid chromatography 를 이용하여 multi-residue pesticides 를 동시분석 할 수 있는 새로운 분석방법을 개발하였다. 시료의 경우 시중에 판매되고 있는 현미녹차에 표준용액을 첨가하여 분석실험을 진행하였고, matrix matching 방법을 이용함으로써 matrix effect 를 감소시켰으며, DSPE sorbent 의 함량에 대한 비교실험을 통해서 최적화된 전처리 방법에 대하여 연구하였다.

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A new luminescent molecular probe for anionic and cationic recognition

정수희

창원대 화학과

A new emissive molecular probe derived from aminophenazine and aminothalazine have been synthesized and characterized by using IR, NMR (^{1}H and ^{13}C), UV-vis and fluorescence 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. The interaction and sensing properties of receptor with different anions were investigated by UV-vis and fluorescence spectroscopy in CH3CN:DMSO (9:1, v/v).

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Multi-residue determination of pesticides in hot pepper by gas chromatography mass spectrometry

안영웅, 이동욱, 이계호

충남대 화학과

최근 들어 생활수준의 향상과 더불어 안전한 먹거리에 대한 국민들의 요구는 갈수록 높아지고 있으며, 양보다는 질에 대한 문제를 생각 할 수 있다. 이러한 시대적 변화에 더불어 식품 중에 잔류하는 농약의 안정성 확보를 위하여 현재 세계 각국에서 농약에 대한 MRL(Maximum Residue Levels)을 지정하여 규제하고 있다.
이 실험에서는 0.1% acetic acid 를 함유한 acetonitrile 을 이용하여 추출 하였고, PSA 를 이용한 Dispersive-SPE 방법을 사용하여 경제적이고, 빠르며 많은 시료에 대해 쉽게 전처리를 할 수 있었다. 또한 GC/MS 를 이용하여 다성분 동시분석을 할 수 있는 새로운 분석법을 개발하였다. 시료에 표준용액을 첨가하여 분석하였으며, matrix 효과를 줄이기 위해 matrix matching calibration 방법을 사용 하였고, 최적화된 전처리 방법과 기기조건을 찾아내었다.
본 실험을 통하여 최적화된 전처리 방법을 개발하여 여러 가지 시료와 분석 물질에 적용하였으며, 동시에 다성분을 분석하는 조건을 개발하게 되었다.

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Insights into distributions of stable isotopic ratios according to burial types of the Joseon Dynasty

강소영, 조은민, 권은실, 지상현

국립문화재연구소 보존과학연구실

In recently human bone remains from the Joseon dynasty period have been investigated vigorously understanding life style, migration of group and regional characterization of the Joseon people. Carbon and nitrogen stable isotope analysis was performed on human skeletal remains of Gimpo (*N*=37) and Anseong (*N*=18) sites in midwestern Korea. In order to determine state of bone preservation, histological analysis was performed using a piece of bone tissue taken from femur, and the atomic C/N ratios for collagen were calculated. Isotopic results show that there are no significant changes between means of male and female within and between sites. The comparison of the data from Anseong site reveals significant differences in $\delta^{13}C$ and $\delta^{15}N$ values among burial types. Human skeletal remains from lime-layered tomb has relatively more elevated mean $\delta^{13}C$ and $\delta^{15}N$ values than them from tomb. This results suggest that social status is one of the decisive factors in determining dietary patterns of the Joseon period.

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Signal enhancement method development using long chain acylation in MALDI-TOF MS

김지수, 김희준

서울대 화학부

Detection of proteins and peptides at low concentration is important in proteomics because proteins perform essential functions at low concentration. We show that long chain acylation of n-terminal is one of the useful methods for MALDI signal enhancement of peptides. The simple long chain acylation reactions enhance the intensity of peaks and improve the limit of detection for most of peptides.

THE KOREAN CHEMICAL SOCIETY

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Ultrasensitive naked eye detection of antigen using coagulation system

권승용, 이미정, 김규원

인천대 화학과

Thrombin is a protein that plays many roles in the coagulation cascade-converting soluble fibrinogen into insoluble strands of fibrin-as well as catalyzing many other coagulation-related reactions. Because of these catalyzing features, thrombin is employed for the immunoassay in our study. Thrombin is conjugated to the secondary antibody-streptavidin complexes. Under the presence of antigen the thrombin complex can be immobilized onto solid surface presenting primary antibody. Upon the exposure of the resulting surface to the solution of fibrinogen, insoluble fibrin is produced on the solid surface. Through this presentation, we demonstrate that the coagulation system enables ultrasensitive naked eye detection of antigen.

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Quantitive Separation of D/L-amino acid modified N,N-Dimethylformamide Dimethylacetal (DMF-DMA) derivative with Quadrupole Time-of-Flight Mass Spectrometry by Applying Kinetic Method

차형래

창원대 화학과

The On-line ESI/QToF-MS by applying Kinetic Method separated D/L-amino acid modified N,N-Dimethylformamide dimethylacetal (DMF-DMA) derivative. we optimized the chemical parameters of 20 chiral amino acids and in order to enhance intensity of cluster ions for ultrasensitive detection. Amino acid formamidene butyl esters are optimally prepared by heating amino acids with dimethylformaide dimethylacetal (DMF-DMA) for 8 minutes at 85°C. I was using Cook's single ratio kinetic method, based on kinetics of competitive unimolecular dissociation of singly charged transition metal ion-bound complexes. Appropriate metal ion and reference ligand were pre-mixed and added to target chiral analyte. These 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 dimeric complex ions, $[M^{II}(A)(ref^{*})–H]^+$ and $[M^{II}(A)(ref^{*})_2–H]^+$. The ratio of two dimeric complex ion abundances for one enantiomer expressed relative to the dimeric fragments of other enantiomer gives chiral discrimination. We developed successive method for rapid quantitative chiral analysis of D/L-amino acid.

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Determination of alkaloids in *Corydalis yanhusuo* extract using solid phase extraction and LC-MS/MS

정은경, *나윤철, **홍종기

*경희대 기초약학과 *한국기초과학지원연구원 분석연구부(서울센터) **경희대 약학과*

Corydalis yanhusuo W.T. Wang has been used as a traditional oriental medicine which showed the therapeutic effects for improving blood circulation, reinforcing vital energy and alleviating pain. Alkaloids were selected as marker compounds in the quality control of *Corydalis yanhusuo* and they can be divided into tertiary and quarternary forms according to their chemical structures. In this study, we developed a clean-up method of nine alkaloids using solid phase extraction (SPE). Their elution patterns on SPE depended greatly upon chemical properties of alkaloids, kind of adsorbents, and the composition of eluents. Two SPE methods (MCX and HLB sorbents) were tested and compared with the eluent solution at the different pH value. MCX as cation-exchange sorbent was shown strong interaction with the quarternary alkaloids so that they were unable to be eluted even with washing solution at high pH. On the other hand, HLB sorbent was shown satisfactory cleanup efficiency of the alkaloids in herbal extract when it washed with NH_3 and water and eluted with MeOH. Alkaloids in purified extract were separated under optimized LC conditions and determined by ESI-MS/MS mode.

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Metabolic profiling of renal cell in rats with chronic renal failure by 1H NMR and LC MS

윤유정

고려대 화학

Metabolite profiling was performed to identify the differences in metabolite patterns by using 1H nuclear magnetic resonance (NMR) and Liquid chromatography- Mass spectrometer (LC ion trap MS) with multivariate statistical analysis technique. In this research, IMCD cells (rat inner medullary collecting duct) with chronic renal failure were characterized using 1H-NMR spectroscopy and Liquid chromatography- Mass spectrometer followed by principal component analysis. We have devised an analytical approach that combines high resolution 1H NMR and LC MS to provide both a large amount of structural information and quantification of a broad spectrum of compounds. This combined approach also simplified sample preparation and reduces the analysis time, making it well-suited for a convenient screening of metabolites. Major endogenous metabolites for IMCD cell contained products of amino acids and organic osmolytes (e.g., sorbitol, betaine, myo-inositol, taurine, and glycerophosphocholine). Many metabolites revealed changes in the profiles of cell metabolites between control and low osmolality group which were influenced by chronic renal failure. Metabolomics of kidney cell based on 1H-NMR spectroscopy and LC MS could provide insight into the effects of osmolality

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Metabolic Studies on Breast Cancer Cell about Metabolic changes by the Expression of an PFKP using ^{1}H NMR Analysis and Multivariate Statistics

이주은

성균관대 화학

Breast cancer is the most common form of malignancy experienced by women. About one in eight women (12.5%) will experience this disease in invasive or noninvasive form in her lifetime. Since the breast cancer is the second largest common cause of cancer deaths, breast cancer has become a major topic of cancer research. Investigating metabolic changes has the potential to reveal crucial enzymatic steps that could be targeted in the drug discovery process. Therefore, it is important to analyze metabolic profile with the regulation of enzymatic activities. NMR-based metabolomics, which combines high-resolution ^{1}H-NMR spectroscopy with multivariate statistics, has been powerful tools to discriminate tumorgenic cell analysis according to their enzymatic conditions. In this study, metabolic profiling using ^{1}H nuclear magnetic resonance(NMR) spectroscopy coupled with multivariate statistics was used to study the metabolic changes between 231-vector and 231-shPFKP cells. This study discusses the regulation metabolisms of glucose in cells by the PFKP(platelet isoform of phosphofructokinase) expression using ^{1}H NMR analysis. Investigating metabolism in cancerous cell has a potential to be diagnosis methods in breast cancer.

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Palatinate Purple dye의 photolytic degradation에 대한 LC/MS 분석

윤여영, *박덕희, *임영희, **조혜성

*(주)LG화학기술연구원 CRD연구소 *LG화학기술연구원 CRD연구소 분석센타 **LG화학기술연구원 CRD연구소*

Palatinate Puple(이하 PP)은 photochromic compound 의 한 종류로서 광변색 필름에 사용되는 dye 이다. PP dye 가 포함된 광변색 필름의 옥외 내후성 테스트를 위해 두 장의 유리 사이에 필름을 접합시켜 자연광에 오랜 시간 노출하였다. 자연광 노출 후의 필름을 유리에서 분리한 후 THF (tetrahydrofuran)로 추출하여 LC/MS 로 분석하였다. 그 결과 PP dye 가 photolytic degradation 되는 것을 확인하였으며 테스트 조건에 따라 degradation product 가 달라짐을 알 수 있었다.

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^{1}H-NMR-Based Metabolomics Study on *Osteoporosis*

김은진

고려대 생명공학과

Osteoporosis is a common and significant health problem. This disease is characterized by a deterioration of the skeleton leading to a high incidence of bone fractures. To research the biomarker of osteoporosis, change of the endogenous metabolites in serum detected from osteoporotic mouse by ovariectomy. In this study, 8 mice were randomly divided into sham-operated(sham) and ovariectomized(OVX) group. Serums were collected from both groups, respectively. The metabolic profiles were investigated using 1H-NMR spectrometry coupled with multivariate statistical analysis such as principal components analysis (PCA). Multivariate statistical analysis showed a significant separation between sham and OVX. The serum of OVX was characterized by the increased level of Alanine, Glutamine, Lactate, Phenylalanine, Pyruvate, Succinate and Valine, and by the decreased level of Glucose. These metabolites influenced of separation both groups. This analytical approach, in combination with chemometrics by multivariate analysis, is expected to offer a diagnostic method of diseases with high reliability and consistent results.

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Lipid Profiling of from Human Plasma by using Nanoflow Liquid Chromatography and Tandem Mass Spectrometry

이주용, 민혜경, 문명희

연세대 화학과

Phospholipids (PLs) are major components of cellular membranes and are classified into molecular species differing in the polar head group and in the acyl chain length along with the degree of unsaturation and Lysophospholipids (LPLs) have one acyl chain in either the sn-1 or sn-2 position of glycerol backbone. PLs and LPLs are related to cell proliferation, apoptosis, and signal transduction, especially some kinds of LPLs and PLs in plasma have been reported as clinically important potential biomarkers of human cancers such as ovarian and colorectal cancer, respectively. However, most of earlier studies were separately made for each category of PLs or LPLs. Since LPLs are derived from the action of phospholipases with PLs, this study focuses to develop an analytical method to profile those species simultaneously so that disease biomarkers can be systematically investigated together with their precursors. Analysis of phospholipids has been carried out with liquid chromatography coupled with mass spectrometry and analysis column was home made capillary column filled with C18 particle. The developed method has been applied to the comprehensive profiling of LPLs and PLs from a human blood plasma sample which results in an identification of 50 LPLs (each regioisomer pair of 6 lysophosphatidylcholines (LPCs), 7 lysophosphatidylethanolamines (LPEs), 9 lysophosphatidic acid (LPAs), 2 lysophosphatidylglycerols (LPGs), and 1 lysophosphatidylserine (LPS)) and 62 PLs (19 phosphatidylcholines (PCs), 11 phatidylethanolamines (PEs), 3 phosphatidylserines (PSs), 16 phosphatidylinositols (PIs), 8 phosphatidylglycerols (PGs), and 5 phosphatidic acids (PAs)).

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Qualitative and quantitative analysis of Phospholipids from Prostate Cancer Cell Lines treated with Allose Using Nano-flow LC-ESI-MS/MS

정래웅

연세대 화학과

Lipidomics defined as the large-scale study of pathways and networks of cellular lipids in biological systems. In lipidomics, it is important to understand the changes in lipid composition and their relative abundance in various biological samples. Phospholipids (PLs) are major component of cellular membrane and asare composed of 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, nano-flow liquid chromatography coupled with electrospray ionization tandem mass spectrometry (LC-ESI-MS/MS) was employed for the analysis of phospholipids mixture in prostate cancer cell line (PrEC, DU145, LNCaP) that were treated with allose. Allose is a monosaccharide present in minute quantities in nature and a rare sugar used as an anti cancer drug (breast cancer or, prostate cancer) without any side effect on human cells. Separation of phospholipids are carried out using a home made reversed phase capillary column and the MS experiment of eluted phospholipids is performed at the precursor scan first and followed by data dependent MS/MS scan. Qualitative and quantitative analysis of PC (phosphatidylcholine), PE (phosphatidylethanolamine), PS (phosphatidylserine), PI (phosphatidylinositol), PG (phosphatidylglycerol) and PA (phosphatidic acid) for the cancer cell lines with or without the treatment of allose are carried out, and the differences of the distribution of the identified PLs are compared in this study.

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Analysis of Phospholipids Using Open-Tubular Capillary Column with a Monolithic Polymer Layer in Capillary Electrochromatography-Electrospray Ionization-Tandem Mass Spectrometry (OT CEC-ESI/MS)

장린, *정원조, 문명희

*연세대 화학과 *인하대 화학과*

Phospholipids(PLs) are major component of cellular membrane as they form double layer structure of membrane and play important roles in signal transduction. While thin layer chromatography (TLC) and HPLC are currently utilized for the analysis of PLs, there is always a need to develop a new method with high speed separation as well as the minimized usage of organic solvents. Currently, capillary electrophoresis is used as an alternative method of separation, but separation of phospholipids with capillary zone electrophoresis can not be obtained by the differences in the length and unsaturation degree of acyl chain of PLs, only by the differences of head groups. In this study, capillary electrochromatography (CEC) has been tested as an alternative method for the separation of phospholipids in combination with on-line ESI-MS-MS. Implementation of OT(Open tubular) column with the help of electroosmotic flow can be an alternative to improve separation in monolithic open tubular capillary electrochromatography(OT-CEC). When used with open-tubular column in this study, we have demonstrated that PLs can be separated not only by head groups, but by the variation in acyl chain. In addition, we developed a simple inexpensive CEC-ESI-MS interface using a coaxial sheath flow in the laboratory incorporated with a simple Tefzel cross. For the performance test of the interface, several peptides were separated and detected by the on-line coupling with ESI-MS. The developed run condition is applied for the separation and characterization of phospholipids extracts from a human urine sample.

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A Comparison Study of Molecular Weight Distribution of Industrially Important Blends of Polysaccharides

무하마드 알리, 문명희

연세대 화학과

Multi-angle light scattering with differential refractive index detector is considered among the most versatile techniques used for the determination of molecular weight distribution of macromolecules. We utilized this instrumentation along with frit inlet asymmetrical flow field-flow fractionation (Fl-AFlFFF) for the comparison of commercially available blends of Sodium Hyaluronate (NaHA) with Hydroxylethyl Starch (HES) and with Carboxymethyl Cellulose (CMC). These blends are utilized in different surgical applications as an anti-adhesive. In the surgical practices, molecular weight distribution is critically important in each application. Enhanced separation by FI-AFlFFF for different sample types provided valuable insight of sample characteristics through MALS-DRI data. Both blends of NaHA with HES and with CMC showed a molecular weight distribution ranging 105-108 g/mol. The NaHA-CMC blends exhibited steeper sigmoidal distribution and a little more compact molecular shape than the NaHA-HES blends. While comparing a raw NaHA and its aggregated formulation, the aggregated one showed very small concentration for higher molecular weight (109 g/mol) and a larger concentration was showed for ambient 105 g/mol. Moreover, it showed to have both compact and linear molecules in its molecular distribution.

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Separation of Glycoproteins with Lectin Immobilized Beads by Flow Field-Flow Fractionation

안지연

연세대 화학과

Glycoproteins are proteins that contain oligosaccharide chains covalently attached to polypeptide side-chains. The failure of such glycosylations can cause various diseases. According to the reports from FDA, many cancer biomarkers are associated with glycoproteins, thererfore characterization of glycoproteins is an important issue in diagnosis of disease. Lectins are specific proteins having a binding affinity to glycoproteins through their sugar moieties and are widely for the identification of glycoproteins. Lectin-affinity chromatography has been utilized to isolate glycoproteins, however only one type of lectin can be used for analysis at a time. In this study, we are developing an analytical method to separate various glycoproteins in serum at once. First, we immobilized different lectins on different sized silica particles. Then these lectin-immobilized beads can be size-separated by flow field-flow fractionation (FlFFF). By using fluorescence labeling to glycoproteins attached to lectins on particle, stained can be quantitatively analyzed. Moreover, size fractionated lectin-immobilized beads can be collected during FlFFF run for the characterization of glycoproteins using shotgun proteomic method. This study was applied to serum sample to validate the developed method.

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A Novel Colorimetric and Fluorescence Sensor for Ascorbic Acid with a Tripodal-Bearing Schiff Base

김현애, 김동완, 김재상

경상대 화학과

The new tripodal bearing Schiff-base groups can act as selective colorimetric and fluorescent sensors for ascorbic acid, which exhibit distinct color changes in the presence of ascorbic acid but show no response to other biological species in 95% DMF+ 5% NaOH aqueous solution (color change light yellow to dark red). More importantly, the sensor displayed significant selective chelation enhanced fluorescence quenching(CHEQ) effect on fluorescence response to ascorbic acid. The proposed sensor was successfully applied for the determination of ascorbic acid in vitamin C tablets

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Quantitative Analysis of Aflatoxin B1 Using SERS-Active Gold Nanostars

추유진, 최남현, 전향아, *이상엽, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과*

Aflatoxin B1 is a well-known carcinogenic contaminant in foods. Thus, it has been extensively used as a biochemical marker to evaluate a degree of food spoilages. Moreover, Aflatoxin B1 is classified as an extremely hazardous compound because of its potential toxicity to a human nervous system. In this study, enzyme immobilized star-shaped gold nanoparticles and Ellman's reagent, dithiobisnitrobenzoate (DTNB), have been used for the quantitative analysis of Aflatoxin B1. High density "hot spots" generation property of star-shaped gold nanoparticles made them efficient SERS inducing probes. For specific targeting of Aflatoxin B1 markers, acetylcholinesterase (AChE) was immobilized on the surface of star-shaped gold nanoparticles. Then, AChE hydrolyzes the acetylethiocholine (ATCh) and this forms thiocholine (TCh), which reacts with dithiobisnitrobenzoate (DTNB) to generate 5-thio-2-nitrobenzoate (TNB, an anion). Quantitative analysis of Aflatoxin B1 was performed by monitoring the SERS intensity variations of TNB. Here, we report a conceptually new SERS-based detection technique using gold nanostars for the quantitative analysis of Aflatoxin B1.

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Analysis of Hindered Amine light stabilizers (HALSs) in Polypropylene with MALDI-TOF MS

임영희, 박덕희, *윤여영, **조혜성

*LG화학기술연구원 CRD연구소 분석센타 *(주)LG화학기술연구원 CRD연구소 **LG화학기술연구원 CRD연구소*

Hindered amine light stabilizers (HALSs) are commonly addedto polymeric materials for the prevention of light-induced degradation of the materials. For anlaysis of the oligomeric or polymeric HALS, MALDI-TOF MS is useful technique because of their large molecular weight. Recently, more than two kinds of HALSs are used to polymer for enhancing the prevention effect. In this study, two kinds of HALSs used in one sample were analyzed. The matrix agent, Dihydroxybenzoic acid, was selected as the optimum matrix for this analysis.

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Analysis of amino acids by carrier-mediated single drop microextraction in-line coupled to capillary electrophoresis

최정미, 김지혜, 최기환, 정두수

서울대 화학부

Carrier-mediated transport was used to extract amino acids in single drop microextraction. 1-Nonanesulfonate served as a carrier and was added to an acidic sample donor solution to form neutral ion-pair complexes with amino acids which were extracted to a liquid membrane and back-extracted to a basic acceptor solution. In the acceptor solution, both the amino acids and carrier have negative charges and the ion-complexes are broken. The amino acids concentrated in the acceptor solution were analyzed by capillary electrophoresis. The effects of the sample pH and extraction time were investigated. The enhancement factors were about 100 times with 20-min extraction.

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Metabolic profiling of renal cell in rats with chronic renal failure by 1H NMR and LC MS

윤유정

고려대 화학

Metabolomics is the measurement of metabolites within an organism, thereby providing valuable insight into the metabolism of cells. In this research, IMCD cells (rat inner medullary collecting duct) with chronic renal failure were characterized using 1H-NMR spectroscopy and Liquid chromatography- Mass spectrometer followed by principal component analysis. We have devised an analytical approach that combines high resolution 1H NMR and LC MS to provide both a large amount of structural information and quantification of a broad spectrum of compounds. This combined approach also simplified sample preparation and reduces the analysis time, making it well-suited for a convenient screening of metabolites. Major endogenous metabolites for IMCD cell contained products of amino acids and organic osmolytes (e.g., sorbitol, betaine, myo-inositol, taurine, and glycerophosphocholine). Many metabolites revealed changes in the profiles of cell metabolites between control and low osmolality group which were influenced by chronic renal failure. Metabolomics of kidney cell based on 1H-NMR spectroscopy and LC MS could provide insight into the effects of osmolality.

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Quantitative selenium determinaiton by HPLC coupled to post-column isotope dilution analysis ICPMS

도미송, 박용남

한국교원대 화학교육과

In this study, a post-column analysis methodology has been applied to carry out the quantitative speciation of selenium in nutritional supplements by HPLC coupled plasma mass spectrometry(ICP-MS). Quantification of selenium was performed by post-column isotope dilution analysis by continuous mixing by a peristaltic pump of an enriched ^{78}Se spike solution the eluent from the column and the mixture was nebulized into the plasma. Finally, after smoothing of the data using moving average in order to reduce the noise level, mathematical corrections were applied to correct for BrH^+. Then, the $^{80}Se/^{78}Se$ isotope ratios were calculated and corrected for mass bias. The total amount of selenium was calculated by integration of each chromatographic peaks. This continuous ID technique was compared with off-line isotope dilution method.

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Development of a novel immunoassay using toner-based microchip

김아란, 최기환, 장서봉, 정두수

서울대 화학부

The toner-based microchip was applied to enhance the immunereaction efficiency. Immunoassay is a valuable method for disease diagnosis. However, immunoassay has several drawbacks; high costs, long analysis times and lack of automation. Even though microfluidic devices can be performed in the rapid analysis times and the automatic control process, it still has difficulty in the wise use of microfluidic immunoassay due to high cost. Recently, the toner-based microchips, which were inexpensive and easy to fabricate compared to the photolithographic process, and its applications were developed. This micro-device is suitable for immunoassay due to disposable device which is required in order to avoid cross contamination. Sandwich immunoassay using a cleavable tag was performed in the microfluidic device. Myoglobin, a marker for muscle injury, was used as a model analyte. After analytes were conjugated to the antibodies immobilized on a particle surface, second antibodies fluorescently tagged were added and complexed with the analytes. Then the tag was cleaved and the solution containing the cleaved tag was analyzed using the microfluidic device. In order to enhance the reliability of immunoassay, a separation step was added. Compared to the immunoassay using a microarray, nonspecific binding effects were reduced due to the separation step. Conjugation and separation was accomplished within 15 min.

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Palladium-carbon nanotube interaction

김자영, 최현철

전남대 화학과

The discovery of fullerenes and carbon nanotubes (CNTs) initiated great interest in the study of non-planar sp2-hybridized carbon nanostructures. These carbon nanostructures can maintain their structural eccentricity and high stability at high temperatures, and even in severe environments, thus allowing them to have many novel electronic, optical, mechanical, and thermal properties. These characteristics allow them to be applied for a catalyst support. 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 hydrodehalogenation. Recently, we prepared palladium-decorated carbon nanotubes (Pd-CNTs) by depositing Pd2(dba)3 on thiolated multiwall carbon nanotube surfaces. The Pd-CNTs effectively promoted the hydrodehalogenation of aryl halides to give the corresponding arenes in 85-99% yield, and exhibited higher activity than that of the reference systems such as Pd2(dba)3 and the Pd2(dba)3/CNT mixture. In this study, we investigated the interaction between deposited Pd and pristine or thiolated multiwall carbon nanotubes.

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Adsorption of malachite green from aqueous solution by dead pine needles

유구용

삼육대 화학과

In this work, the dead pine needles was evaluated for its ability to remove malachite green from an aqueous solution in a batch process. Equilibrium studies were conducted in the range 5.0 - 12.5mg/L initial malachite green concentration, 2 - 9 solution pH and at temperature of 25°C. The experimental data were analyzed by the Langmuir, Freundlich, Temkin isotherm models. Equilibrium data were fitted to the Freundlich and the Langmuir model. The maximum adsorption capacity of malachite green on dead pine needles in aqueous solution was evaluated. The dimensionless separation factor RL revealed the favorable nature of the isotherm of the malachite green-dead pine needle system.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Quantitative analysis of selenomethionine in human serum by HPLC-ICP MS

정지선, 도미송, 박용남

한국교원대 화학교육과

In human serum, most of the selenium present is known to be protein-bound and to occur in the form of two seleno-amino acids. One of them, selenocysteine is considered to be forms of the glutathione peroxidases (GPx) and selenoprotein P (SeP). Selenomethionine is supposed to be incorporated randomly into methionine-containing proteins, selenoalbumin (SeAlb). Because SeAlb is not synthesis genetically encoded, it can play the role of a potential bio-indicator of selenium status. The purpose of this study is quantitative analysis of selenomethionine in Korean human serum by reversed phase-HPLC ICP MS. The quantification of SeMet is carried out by the method of standard additions. A serum sample is enzymatically digested with protease ⅩⅣ and lipase. Selenomethionine concentrations in Korean human serum is 29.63μg/L. And Total selenuim in Korean human serum by external calibration is 83μg/L.

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대용량 전처리법을 이용한 수질 시료 내 극미량 다이옥신의 분석

박덕희, 윤여영, 임영희, 조혜성

LG화학기술연구원 CRD연구소

수질 시료 내 극미량의 다이옥신을 정확하게 분석하기 위해서는 많은 양의 시료가 필요하다. 5 L 이상의 대용량 수질 시료를 액액 추출법(Liquid-Liquid extraction)으로 추출하기 위해서는 추출을 반복 수행하고 추출물을 여러 번 농축하는 과정을 거쳐야 한다. 이런 방법으로 추출할 경우 유기 용매의 사용량이 늘어나고 많은 농축 과정을 거치기 때문에 안정적인 회수율 확보에 어려움이 있다. 이러한 어려움을 극복하기 위한 대안으로 고상 추출법 (Solid-Phase extraction)을 도입하였다.대용량 추출을 위한 고상 추출 장치를 설치하고 회수율 측정으로 추출 효율을 검증하였다. 대용량(7 L) 추출 시 회수율은 17 종 congener 모두 50~120% 이내로 분석되었다. 저농도 수질 시료를 액액 추출법 (500 mL)과 대용량 고상 추출법 (7L)으로 전처리 하여 분석한 결과 검출된 congener 들의 정량 값이 유사하였다. 또한 500 mL 전처리시 검출되지 않은 몇 개의 congener 들이 대용량 전처리를 통해서는 정량 되는 것을 확인하였다.

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Developments of H^1/N^{15} Solid-state NMR Probe for Structural Studies of Membrane Proteins in Aligned Bicelles

박태준, 김지선, 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. A lipid bilayer provides the protein with a physical and chemical environment most similar to a natural membrane, but the large size and slow tumbling of lipid bilayer require the use of solid-state NMR methods. Solid-state NMR experiments on lipid bilayers 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. The orientational restraints from membrane proteins in a lipid environment could be obtained by H^1-N^{15}heteronuclear dipolar coupling solid-state NMR experiments, PISEMA or SAMMY. Most of biological lipid samples have high dielectric property due to containing large amounts of water and salts. This electrical property cause a loss of probe efficiency from severely reducing the probe Q-factor and significantly shifting the tuned frequency down. Moreover, these biological samples are readily heated and destabilized during radio frequency irradiation. For these reasons, a specific probe with high efficiency and high capability is required to study these biological samples by using solid-state NMR, and several probe designs have been developed in a recent research to improve the probe efficiency. Here, we present the optimized design, construction, and efficiency of a 400 MHz wide-bore H^1-N^{15}solid-state NMR probe with 5-mm solenoidal rf coil for high power, multi-pulse sequence experiments, such as 2D PISEMA or 2D SAMMY. This probe provides short pulses, high power capability, and good rf homogeneity. H^1-N^{15}2D SAMMY spectra from a single

crystal and membrane proteins in oriented phospholipid bicelles was successfully obtained by using this home-built solid-state NMR probe at 400 MHz.

대 한 화 학 회
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Structural investigations of manganese-rich $0.3Li_2MnO_3 \cdot 0.7Li[Mn_{0.7}Ni_{0.2}Co_{0.1}]O_2$ by in situ X-ray absorption fine spectroscopy

송혜영, 서가영

울산대 화학과

X-ray absorption fine spectroscopy (XAFS) is a very useful tool to investigate the structural and electronic properties of this compound. Manganese-rich oxides are alternatives to cobalt-based oxides due to low cost and high safety as positive electrodes in Li-ion batteries. $0.3Li_2MnO_3 \cdot 0.7Li[Mn_{0.7}Ni_{0.2}Co_{0.1}]O_2$ was investigated in practical Li-ion intercalation electrodes used for Li-ion batteries by applying in situ XAFS, which make to study the atomic and electronic structure of these materials and understand the changes occurring upon cycling.

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Fixation of silica packing at the entrance of microchannels of fully packed CE microchip by ellectroless siver plating

박종만, 오혜진

건국대 화학과

A method of fixation of the submicron silica packing at thhe entrance of the microchannels of a fully packed capillary electrophoresis microchip is developed by utilizing electroless silver plating technique. Recently we have reported fully packed capillary electrophoresis microchips showing good CE separation characteristics with few milimeter separation channel. The microchannels were fully packed with monodisperse silica colloidal particles, which can be utilized as built-in nanofilters and stationary phase supports after derivatization. However the silica packing at the microchannel entrances can be destroyed by erosion during potential application. To avoid the erosion problem the silica packing at the channel entrances was fixed and stabilized by silver electroless plating technique. The details of silver electroless plating and the surface morphologies of the silver plated silica packing wll be demonstrated.

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Analysis of Blend ratio of Polyethylene/Poly(ethylene-co-vinyl acetate) blends

송신헌, *신은미

*LS전선 분석기술그룹 *LS전선 중앙연구소*

Over past a few decades, polyethylene (PE) and poly(ethylene-co-vinyl acetate) (EVA) have been widely used in many industries due to their exceptional thermal, mechanical and physical properties.

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Simultaneous determination of monensin and salinomycin in animal tissues, milk and egg by Liquid chromatography-tandem mass spectrometry

이종혁, 마경나, 황효진, 조현우, 명승운

경기대 화학과

Monensin and salinomycin are used in veterinary applications as coccidiostats for poultry and livestock and as growth promoters for ruminants to increase feed conversion efficency. Analytical method based on liquid chromatography-tandem mass spectrometry (LC-MS/MS) for determining in animal tissues, milk and egg were presented. The method included extraction with acetonitrile followed by a clean-up on a silica cartridge. Chromatographic separation was achieved on C18 column (2.1×100 mm, 3.5 μm), using isocratic elution with water and acetonitrile (94:6), which one containing 0.1% formic acid. After HPLC separation, quantification and qualification were performed by electrospray ionization (ESI) - tandem mass spectrometry. As a result, the limit of detection (LOD) and limit of quantification (LOQ) were different for the various analyte/matrix combinations but were in all cases below 0.0018 and 0.0059 mg/kg, respectively. The established method can be used to determine mg/kg levels of monensin, salinomycin from the tissues sample.

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Determination of Amprolium, Decoquinate and Dicyclanil in animal tissues by HPLC/UV

김병주, 함현선, 홍지연, 명승운

경기대 화학과

To increase production of livestock products, some livestock and poultry farms may use coccidiostats (amprolium and decoquinate) and insecticide (dicyclanil). Analytical method for a determination of vertinary medicine (amprolium, decoquinate and dicyclanil) in animal tissues (cattle, chicken and lamb) by HPLC/UV were established. Samples were extracted by the SPE (Solid-Phase Extraction) that used a HLB (Hydrophilic-Lipophilic Balance) cartridge and ACN. Chromatographic separation was achieved C18 column (4.6×250mm, 5μm), using gradient elution with 20mM HFBA, MeOH or MeOH : ACN (1:1.8). The calibration curve from spiked blank matrix showed good linearity (above r^2=0.995) in the concentration range of 0.051-12.0 mg/kg. Limits of quantification (LOQ) were the range of 0.015-0.13 mg/kg. In case of amprolium for cattle, LOD was 0.04 mg/kg, precisions were the range of 3.1-6.1 % and accuracy was the range of 98.3-101.9 %. The developed method can be used to determine under the MRL (Maximum Residue Limits) level of vertinary medicine.

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The Analysis of Spectinomycin residues using LC/ESI-MS/MS in Swine, Cattle and Chicken tissue

박미선, 김유진, 이진주, 명승운

경기대 화학과

In veterinary medicine, spectinomycin is used therapeutic agent of bacterial respiratory and enteric infections for animal. In this study, spectinomycin was extracted from swine, cattle and chicken tissue using solid-phase extraction(SPE) employing a HLB cartridge with 5% trichloroacetic acid in 20mM HFBA. Liquid chromatography/tandem mass spectrometry (LC/MS/MS) for the analysis of spectinomycin from animal tissue was presented. Spectinomycin was detected on a C18 (2.1×100 mm, 3.5 μm; waters, U.S.A.) column using a mobile phase of 20mM HFBA in water and acetonitrile. A linear correlation observed in the calibration curves for animal tissues over the range of 0.01～3.0 mg/kg showed above r2=0.995. Absolute recovery was the range of 30.0%～50.0%. Limit of detection (LOD) and limit of quantitation (LOQ) were the range of 10.0～30.0 ng/kg and 17.0～35.0 ng/kg respectively. The established method can be used to determine low ng/kg levels of spectinomycin residues from swine, cattle and chicken tissue.

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Electrokinetic chromatographic separation of aniline-derivatives with a monodisperse silica colloid packed CE microchip

박종만, 김문희

건국대 화학과

A fully packed electrochromatographic microchip was prepared by packing monodisperse silica particles in the microchannels of the microchip. Capillary action and self assembly behavior were utilized to pack the microchannels patterned cyclic olefinic copolymer substrate with the silica particles. After cover bonding and reservoir fabrication the chip was tested for the separation of aniline derivatives by electrokinetic chromatographic technique. Basic borate buffer solutions with sodium dodecylsufate(SDS) were used to characterized separation behavior. The separation characteristics were studied in terms of pH of the solution, buffer concentration, SDS concentration, separation voltage as well as separation channel length. Five aniline dedrivatives tagged with fluorescamine were separated successfully withb optimized separation conditions.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

In-depth profile analysis of nano multilayer coatings on a glass by pulsed radio-frequency glow discharge optical emission spectroscopy

윤장희, 원미숙

한국기초과학지원연구원 부산센터

Pulsed radiofrequency glow discharge optical emission spectrometry(Pulsed-RF-GD-OES) was used for the in-depth quantitative analysis of a Ni/Ag multilayer on the glass substrate. The technique resulted in a rapid and accurate depth profiling of the multilayer, down to the nanometer range. The analytical parameters were optimized for the in-depth quantitative analysis of a Ni/Ag multilayer on the glass substrate. The GD depth profilings with or without using the pulsed RF technique were compared to confirm the validity of the pulsed RF technique. SEM image showed the thicknesses of the Ni/Ag multilayers. The findings indicate the use of RF-GD-OES in surface analysis of this type is an adequate and promising analytical tool for this challenging application.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Catecholamines Separation with Stacking by Constant-Voltage Mode Counter-Pressure ITP-CZE with Boundary Control

장서봉, 정두수

서울대 화학부

Isotachophoresis (ITP) is one of the powerful sample stacking methods that samples are stacked between leading and terminating electrolyte boundaries. We present a constant-voltage mode counter-pressure ITP-CZE (CCIC) method which combines electrokinetic injection and transient ITP (TITP). Counter-pressure is applied to the opposite direction of isotachophoretic moving boundary and this enables position control in capillary to hold the boundary during stacking and reserve enough length for CZE separation. This method is applied in commercial capillary electrophoresis (CE) equipment to obtain high enrichment and better separation resolution. Counter-pressure is independent of other separation parameters and it can provide quite simple control. The analytes used in this experiment are three catecholamines; dopamine, epinephrine and norepinephrine. Catecholamines are important biomarkers which has various roles in biological system. Without any derivatization, three catecholamines are analyzed with UV-Vis detection. Using field-amplified CCIC (fCCIC) method, we got 34000 times sample enrichment compare to CZE analysis. Compare to conventional TITP, we got 150 times sample enrichment and better resolution due to the position control. The limit of detection for 30 minute stacking fCCIC is 2 nM. CCIC can be widely used in conventional CE with high concentration enrichment and good resolution when an ITP condition with electrokinetic injection is possible.

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Lateral flow Immunoassay with Chemiluminescent Signal Band

고혁, 박민, 이주경, 김조일, *변재철

*연세대 신소재공학과 *연세대 신소재공학부*

Lateral flow immunoassay (LFI) has been widely used for the detection of biomarkers for diseases1) microorganisms2) and toxins3). Recently, the discoveries in genomics, functional genomics, and proteomics have been reported new biomarkers for medical diagnosis. Usually, such new biomarkers require of far lower detection limits in comparison with that of the conventional LFI methods of approximately 1 -10 ng/ml4) So, the CL by the reaction between horseradish peroxidase (HRP) and luminol is applied for the improvement of the sensitivity of the LFI method and the test result is displayed by using a signal band with luminescence instead of the color change. The feasibility of the new LFI with a CL signal band was presented by the detection of horseradish peroxidase (HRP) as a model analyte. Next, the applicability of this new method to sandwich-type immunoassays was demonstrated by the detection of human chorionic gonadotropin (hCG), and the sensitivity was determined to be improved as much as 106-fold in compared to the conventional LFI based on colored gold-colloids.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Electrocatalytic reduction of H2O2 on a multi-wall carbon nanotube modified electrode

정유나, 최현철

전남대 화학과

Many analytical methods have been developed for the detection and quantification of H2O2. Among them, titration, spectrophotometric, fluorometric, chemiluminescent, and chromatographic techniques are well known. However, electrochemical methods have emerged as preferable, owing to their relatively low cost, efficiency, high sensitivity, and ease of operation. In this work, we prepare the multi-walled carbon nanotube (CNT) supported palladium nanoparticles, the fabrication of CNT modified electrode, and its application in the electrocatalytic reduction of H2O2 in 0.1 M pH 7.4 phosphate. Electrocatalytic behaviors were also compared with the commercial Pd-carbon black system. The as-prepared CNT modified electrode shows excellent electrocatalytic properties, and have great potential for applications in electrochemical detection.

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EDC를 이용한 peptide C-terminal 구분법

신만섭, 김희준

서울대 화학부

EDC 는 카르복실 그룹과 아민을 연결하는 coupling reagent 를 사용된다. 카복실그룹에 반응성은 우수하나 펩타이드 내에서는 C-terminal 에만 작용하는 선택성 부분에서는 사용할 수 없었다. 그러나 우리는 kinetics 및 반응 조건의 변화를 통해 선택성을 확인하는 연구를 수행하였다.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Electrochemical ELISA by using diamond-like carbon (DLC) microelectrode

김조일, 박민, 이주경, 고혁, *변재철

*연세대 신소재공학과 *연세대 신소재공학부*

A diamond-like carbon (DLC) microelectrode was applied for diagnosis of RA (rheumatoid arthritis). In this work, oxidized 3,5,3',5'-tetramethylbenzidine (TMB) was quantified by amperometry instead of optical density measurement. Quantification was carried out by using a boron doped DLC microelectrode and cyclic voltammetric analysis method without quenching step which uses sulfuric acid. For the RA diagnosis, the cut-off value was determined by considering the sensitivity as well as the selectivity of the analysis. The test results demonstrate that electrochemical ELISA using DLC microelectrode was feasible for the RA diagnosis

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

Development of a high performance cell activity measurement system for analysis of cell-light interaction

홍혁기, 최연식, 조영창

전자부품연구원 메디컬IT융합연구센터

광 기반 의료용 치료기술은 의료계에서 활발하게 사용되고 있다. 이러한 치료기술은 과거 UV 램프나 열선 램프를 사용하였으나 최근 반도체 기

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발표종류: 포스터, 발표일시: 금 15:00~17:00

ECL sensor for pyrophosphate

배세원, 홍종인

서울대 화학부

The conventional PPi detection is based on fluorescent or bioluminescent approaches which necessarily accompany bulky and expensive analytical instruments. Considering the important and ubiquitous roles of PPi in biology and environment, there is an urgent need to develop an ECL sensor that would enable highly sensitive and selective detection of PPi with minimizing additional equipments (without light source and additional separation tools). Herein, we demonstrate a new proof of concept for ECL-based pyrophosphate (PPi) sensing, where the emission intensity is changed by electrochemical turn-on. The presence of PPi is confirmed from the change in the intensity of green ECL generated from the former when PPi is selectively recognized by the latter. During PPi recognition, changes of ECL intensity are caused in the electronic states of the receptor, and this stimulates the attenuation of ECL.

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A study on GC/MS determination of isocyanates by using derivatization technique after converting into diamines

성준현

식품의약품안전평가원 첨가물포장과

Isocyanates are used predominantly in the production of polyurethane polymers, elastomers, flexible and rigid foams. Especially, 2,4-toluene diisocyanate(2,4-TDI), 2,6-toluene diisocyanate(2,6-TDI), 4,4'-methylenediphenyl diisocyanate(4,4'-MDI) and hexamethylene diisocyanate(HMDI) are mainly used as a monomer in the industry application. In view of the human health, a rapid and sensitive method of analysis is needed to detect them in environmental samples or food packaging. In this study, the method to determine these isocyanates was validated by gas chromatography/mass spectrometry(GC/MS). Isocyanates were derivatized with ethyl chloroformate after hydrolyzing into corresponding amines, 2,4-toluene diamine(2,4-TDA), 2,6-toluene diamine(2,6-TDA), 4,4'-methylenediphenyl diamine(4,4'-MDA) and hexamethylene diamine(HMDA), under the acidic condition. All the derivatives show good chromatographic performance and sufficient sensitivity under the analytical condition using HP-1 capillary column. It is considered that the developed method can be applied to the determination of isocyanates in environmental samples and polyurethane products.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Analysis of Arsenic Compounds Using Single Drop Microextraction In-line Coupled with Capillary Electrophoresis

Cheng Khley, 정두수

서울대 화학부

Sensitive analysis technique of the arsenic compounds based on single drop microextraction (SDME) in-line coupled with capillary electrophoresis (CE) was developed. With this technique, preconcentration and separation was performed in a single run. The analytes were toxic compounds including inorganic As(III), As(V), and dimethylarsinic acid (DMA), monomethylarsonic acid (MMA). Three–phase SDME have used the partitioning of the analytes between the aqueous phase and the organic membrane. However, negative charge of the arsenic compounds prohibited the partitioning to the organic membrane. In order to alleviate this problem, positively charged Aliquat 336 were added the organic membrane as a carrier. The carrier and arsenic compounds formed ion-pair complexes, thus partitioning the arsenic compounds into the organic membrane. The arsenic compounds in the organic membrane are back-extracted to the basic acceptor phase simultaneously with the counter-transport of the hydroxide ions. After extraction, the acceptor phase is injected and arsenic compounds are separated by CE. The effects of extraction parameters including the concentration of the carrier, the pH of the acceptor phase, and the ionic strength of the donor phase, and extraction time were investigated. The enrichment factors were from 13 to 140 with 5-min SDME. In addition, this technique was successfully applied to the environmental samples.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Gas Chromatography/Mass Selected Detecter 를 이용한 Cable내 시스체의 유기첨가제 분석에 의한 내한성의 차이 연구

유정석, 신은미

LS전선 중앙연구소

Gas Chromatography/Mass Selected Detecter 를 이용한 Cable 내 시스체의 가소제 등 유기첨가제를 분석 비교 연구한 결과 유기첨가제의 성분과 함량의 차이가 내한성의 차이에 큰 영향을 줄 수 있음을 알았다

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Silver(I) selective PVC membrane electrodes based on Schiff base 2,2'-(1E,1'E)-(1,1'-binaphthyl-2,2'-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol complex as an ionophore

이은희, 정은선, 전승원

전남대 화학과

The potentiometric sensor based on Schiff base 2,2'-(1E,1'E)-(1,1'-binaphthyl-2,2'-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol has been synthesized and explored as ionophore for preparing PVC-based membrane sensors selective to the silver (Ag+) ion. Potentiometric investigations indicate high affinity of this receptor for silver ion. The best performance was shown by the membrane of composition (w/w) of ionophore: 1 mg, PVC: 33 mg, o-NPOE: 66 mg and KTpClPB as additive were added 50 mol% relative to the ionophore in 1 ml THF. The sensor works well over a wide concentration range 1×10^{-2} to 1.0×10^{-6} M by pH 6 at room temperature (slope 60.99 mV/dec.) with a response time of 4 seconds and showed good selectivity to silver ion over a huge number of interfering cations. It could be used successfully for the determination of silver ion content in environmental and waste water samples.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

Development of a superoxide sensor based on modified electrode by MWCNT-Pd and superoxide dismutase

김슬기, 유정민, 정해상, 김대근, 전승원

전남대 화학과

Superoxide produced in vivo plays various pathphysiological and physiological roles, and thus it is of great importance and value to evaluate quantitatively dynamic changes in superoxide concentration. We thus aimed at developing MWCNT-Pd and superoxide dismutase (SOD) immobilized sensor. Furthermore, the wide linear range, low detection limit, good reproducibility and excellent storage stability were obtained from amperometric response. These results show that the proposed electrode displays better electrocatalytic activity compared to the previously reported palladium modified electrodes toward dismutation of superoxide.

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Detecting Hydroquinone and Catechol using Glassy Carbon Electrode modified with MWCNTs-Palladium nanoparticles and PEDOP

Orogzodmaa Naranchim, 김슬기, 전승원

전남대 화학과

An effective sensor (GCE/MWCNTs-Pd/PEDOP) for the determination of Hydroquinone (HQ) and it's isomer Catechol (CA) were synthesized and compared with poly 3,4-Ethylenedioxy pyrrole (GCE/PEDOP) and Multi Walled Carbon Nanotubes Palladium nanoparticle (GCE/MWCNTs-Pd) sensors. The modification could be made by simple processes on Glassy Carbon Electrode (GCE) with MWCNTs-Pd covered by PEDOP in 0.05M TBAP/MeCN solution system. A well defined peak potential evaluation (+0.05V versus Ag/AgCl) of oxidation of Hydroquinone to Quinone and electrochemical reduction back to Hydroquinone were found by Cyclic Voltammetry (CV) in Phosphate Buffer Solution (PBS) at pH 7.4 (different pH-PBS comparison experiments were also carried out with concentration of 100μM and 200μM of HQ and CA). Also peak current values were increasing linearly with increasing Hydroquinone contents. Moreover, good reproducibility, excellent storage stability, wide linear range and low detection limit were determined by using Differential Pulse Voltammetry (DPV) and amperometric responses and makes it promising candidate for determination of Hydroquinone (HQ) as sensor.

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발표코드: **ANAL.P-151**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

New colorimetric chemosensors based on Schiff base for the detection of Cu2+

정은선, 이은희, 전승원

전남대 화학과

A novel chemosensor, based on base 1,2-bis(E-2-hydroxy benzylideneaminoanthracene-9,10-dione containing anthraquinone as chromogenic signaling submit as chromophore, has been developed for the colorimetric determination and visual detection of copper(II) ions. This molecular sensor exhibits substantial color changes upon complexation with these metal cations in acetonitrile and dimethyl sulfoxide mixture solutions. Well-defined color change in the visible region of the spectrum was observed upon addition of copper ion in DMSO/MeCN (1:9) solution of the receptor.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Studies on Convergent Peptide Ligation

권윤진, 방두희

연세대 화학과

The key technique of protein synthesis is native chemical ligation which ligates unprotected peptide-thioester and a cystein-peptide. Here we investigate convergent chemical ligation for X-Cys ligation sites, where X is V,G,A,. We synthesized LYRAX-thioester peptides and CLAFKX-thioester peptides. Then we perfomed combinatorial ligation reactions between them to show optimal solution for the convergent peptide ligation strategy.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Preparation of Gene Carrier Using a Surface Modified Polydiacetylene Liposomes and Its Application to biosensor

안난영, *임강혁, *최혜, *최준식

*충남대 생화학과 *충남대 생화학과*

Polyethylenimine(PEI) has been used for non-viral gene carrier because of its cationic property and DNA condensing ability. Polyethylenimine with high molecular weight has exhibited high gene delivery efficiency, but its toxicity is high, too. Polydiacetylene(PDA) liposomes are made of diacetylene lipid monomers. These liposomes are polymerized through the ultraviolet irradiation and they undergo chromic change by various environmental stimuli. Their specific properties have been widely studied as chemical or biological sensor systems. Also, these liposomes can be used for gene or drug carriers. In the present study, we synthesized polyethylenimine-modified polydiacetylene liposomes as liposomal vector for gene delivery. We confirmed these liposome's properties and performed transfection assay. As the result, these liposomes showed some gene delivery efficiency and low toxicity. The study indicate that polyethylenimine-modified polydiacetylene liposomes is expected to be an efficient gene carrier system with low toxicity.

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A Single Ligand AFM Tip through Picking a DNA and Ligation of a DNA-Peptide Conjugate

이지하, 김정숙, *류성호, 박준원

*포항공과대 화학과 *포항공과대 분자생명과학부*

Atomic force microscopy (AFM) is widely used to measure interaction forces between biomolecules for its high lateral resolution and superior force sensitivity. It is important to chemically immobilize biomolecules on a AFM tip, so our group has used a cone-shaped dendron which ensures homogeneous and sufficient spacing about 5-7 nm to minimize steric hinderance between modified biomolecules. For more accurate analysis, we needed to ensure single biomolecule interaction. Therefore we developed a single ligand tip through picking a DNA and ligating a DNA-peptide conjugate. DNA and peptide are covalently conjugated to GMBS which is a hetero-bifunctional cross-linking reagent. We expect to obtain the high accurate distribution force map of the formyl peptide receptor (FPR) on the cell surface through this single ligand tip.

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Interaction between AKR2 and OEP7 with Force-based AFM

이재은, 김일홍, 박준원

포항공과대 화학과

In plant cell, Arabidopsis ankyrin repeat protein (AKR2) is a cytosolic mediator to recognize the targeting signal of Arabidopsis chloroplast outer envelope membrane protein (OEP7) and can transport OEP7 to the chloroplast. We measured specific interaction forces between AKR2 and OEP7 with AFM to observe the recognition point of AKR2 and to demonstrate the signal network of the chloroplast outer membrane. The quantitative analysis of protein-protein interaction can show whether AKR2 is specific mediator for transmembrane domain/C-terminal positive region (TMD/CPR)-type targeting signals of OEP7 or also recognizes others.

THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Lyophilized Microtubules for Studying the Structure of Microtubule Stabilizing Agents

백윤기, *타스리마펄도우스, *이상학

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Microtubule stabilizing agents are small organic compounds that promote the polymerization of tubulin and stabilize the microtubules. Many of these compounds are potent antitumor drugs and several have found wide use in the clinic which include taxanes, paclitaxel, and epothilones. A detailed knowledge of the atomic structure of protein/ligand complexes is desirable to understand the mechanism of action of the drugs and to help optimize their activity or to identify new leads. In this study, we have developed protocols to prepare lyophilized microtubules for studying the structure of microtubule stabilizing agents in solid states. Electron microscopy data show that taxol-stabilized, lyophilized microtubles have the same morphology as epothilone-stabilized, lyophilized microtubules. Relevant experimental parameters were optimized and solid-state 13C CPMAS NMR spectra were acquired from lyophilized microtubules with a tubulin content of 15 and 40 w%, respectively, of the buffer medium.

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The studies of interaction between each domain of human RIG-I and AIV NS1

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The first line of antiviral immune defense in higher eukaryotes is dependent upon a rapid activation of latent transcription factors to drive the expression of antiviral genes and the production of α- and β-interferon (IFN). IFN-stimulated gene products limit virus replication and serve to modulate the immune response. So expression of IFN is very important for our antiviral immune defense. Retinoic acid-inducible gene I (RIG-I) is known as an intra-cellular sensor of virus infection. RIG-I senses various types of viruses, such as Influenza virus and Hepatitis C virus. They bind to viral dsRNA or 5'pppssRNA, and then change their structural conformations into active form and IFN pathway is stimulated. RIG-I is imperative for induction of IFN-I in response to Influenza A virus (IAV). But NS1 protein of AIV suppresses induction of INF-I by targeting and inactivating the RIG-I-dependent signaling pathway. So we studied the interaction between RIG-I and NS1 of Avian Influenza virus (A/HK/483/1997 (H5N1)) by Enzyme Linked Immunosorbent Assay (ELISA). Our results show that RIG-I full-length specifically binds to the NS1 of AIV (K_D = 40 nM) in the presence of polyI:C, but does not bind in the absence of RNA. And we have shown that helicase domain of RIG-I is responsible for NS1-binding region by ELISA. Acknowledgment: This work was supported by Seoul R&BD Program (10580).

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Quantitative isotopic nitrocellulose filter binding assays: SARS CoV helicase-nucleic acid interactions

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Helicases play essential roles in viral life cycle and translocate along nucleic acids using the energy of NTP hydrolysis. The ability of a helicase to bind single-stranded nucleic acid is critical for nucleic acid unwinding. As a step to understand the mechanism of unwinding, DNA binding properties of the SCV helicase were investigated by filter binding assay.Nitrocellulose-filter binding is a powerful technique commonly used to study helicase-nucleic acid interactions. Nitrocellulose-filter binding is used extensively to investigate equilibrium binding and kinetic properties of helicase-nucleic acid complexes because of the preferential retention by nitrocellulose of helicase and helicase-DNA complexes but not of free DNA. By using radiolabeled DNA, the amount of DNA complexed with helicase in a solution can be quantitated by filtering it through nitrocellulose and measuring the amount of radioactivity retained on the membrane.We also performed the filter binding assay with ssRNA of different lengths and studied high binding conditions for helicase-nucleic acid binding. The results show that SCV helicase bind nucleic acid without any preferences and its binding affinity has low retention efficiency.Acknowledgment: This work was supported by Seoul R&BD Program (10580).

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Assessment of Cell-Surface Interaction on Physicochemically Modified Surfaces

PRAKASH CHANDRA, Mahto Sanjeev Kumar, 이석우

공주대 화학과

In this study, we describe the most expected behaviour of cells on the modified surface and the correlation between the altered substrates and the response of cells. The physicochemical characteristics of materials such as their stiffness, surface energy, topography, and composition, play an essential role in the adhesion and proliferation of cells. Glass and polymer substrates were altered with plasma oxidation, UV treatment, and surface coating with SAMs materials and ECM. BALB/3T3 fibroblast cells were cultured on the different surfaces with distinct wettabilty, and the growth rates were analyzed. Finally, we found the optimum conditions for the adhesion and proliferation of cells on the modified surface. This study will provide the insight into the cell-surface interaction and contribute to tissue engineering applications.

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Study on the interaction between the Plasmodium vivax circumsporozoite protein and Human importin alpha 3

이성환, 송경미, 최성진, 전위정, 정의영, 조헌호, 반창일

포항공과대 화학과

Plasmodium, malarial parasite, is parasitic on the hepatocyte to prepare next infection onto the erythrocyte making thousands of merozoites. The circumsporozoite (CS) protein has a central role in this stage. Since the CS protein has nuclear localization signal (NLS), it can be introduced into the nucleus by the importins, especially importin alpha 3, and competed against the NFκB resulting inhibition of the expression of many genes that are related with the NFκB. Recently, it has been reported that the CS protein from Plasmodium yoelii and importins seem to directly bind each other. However, Plasmodium yoelii is not a human malarial parasite, and also they could not be sure the lack of adapter molecule. Therefore, more specific researches are still necessary to investigate for influence on human malaria disease. In this study, we purified the human malarial CS protein from Plasmodium vivax (PvCSP) and importin alpha 3 (Impα3). In order to verify the direct interaction, we investigated in vitro binding assay using native SDS-PAGE and surface plasmon resonance (SPR). It showed that interaction of PvCSP and Impα3 is direct, and dissociation constant is 15.4 nM. In the case of SPR studies, interestingly, we could not observe the interaction of two proteins when Impα3 was immobilized on NTA-chip. Based on these results, we suggest that PvCSP may enter the major porket of Impα3 which is locating near its N-terminal region instead of minor porket.

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Fabrication and Applications of Biomimetic 3D-Artificial Membranes

박지은, *하태환

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최근 들어서 바이오칩의 응용 가능성이 다양하게 대두되면서 소형화 또는 집적화된 칩 표면에서의 생체분자 반응의 이용을 위한 기술 및 기법들이 다양하게 개발되고 있다. 이러한 연구를 위해서 MEMS(Microelectromechanical systems) 기술을 바이오산업에 적용하려는 움직임이 거세게 일고 있다. 본 연구에서는 인공지질막 형성을 위한 지지체로서 KOH 에 의한 실리콘 이방식각을 통해, 수 um 스케일의 규칙적인 돌기패턴의 PDMS 구조를 제조하고 그 위에 지질막을 형성함으로써 실제 세포모델과 비슷한 환경을 만들 수 있었다. 이렇게 제조된 인공 세포막을 이용해 항생 펩타이드에 의한 인공지질막에 미치는 영향 및 지질막과 DNA, 단백질 등과 같은 바이오분자들간의 상호작용을 연구하였다. 새로운 인공지질막 형성을 통해 생화학, 생물학, 신경과학 등에서 생체분자간의 상호작용을 연구하는데 큰 도움이 될 것으로 기대된다.

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Magnetic bead-based method of screening double-strand DNA binders

조헌호, 송경미, 전위정, 정의영, 이성환, 최성진, 반창일

포항공과대 화학과

Separation techniques using magnetic particles have been widely used for high-throughput screening of dsDNA binders. This method is pretty simple, and does not require a large and expensive machinery system. Since the reaction and purification processes of the screening are carried out just in a single tube, using an external magnet can reduce the amount of unnecessary material and shorten the experimentation time. Such advantages can make it possible to simply screen effective target materials from within large pools of synthetic chemicals obtained from combinatorial chemistry. We designed a high-throughput screening method for DNA binders using dsDNA-modified magnetic particles. Hairpin DNA immobilized on magnetic particles was used to select only dsDNA binding materials, and then loaded candidate materials on the modified magnetic particles could be separated in a short time using the general external magnet. With these processes, only dsDNA binders were sorted out from mixtures, and their relative binding strengths were verified by the melting temperature (Tm).

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Studies on the functional properties of recombinant SDF-1

전위정, 송경미, 정의영, 이성환, 최성진, 조헌호, 반창일

포항공과대 화학과

The SDF-1 protein is a homeostatic chemokine with multiple roles in cell homing, tumour metatasis, angiogenesis and tissue regeneration after acute injuries. The N-terminal residues of SDF-1 participate in the binding and activation of the target receptor. In particular, Lys1 and Pro2 are directly interact with the CXCR4 receptor. DPPIV/CD26 selectively cleaves dipeptide from N-terminus of substrate containing proline or alanine in second position. In addition, a slow remove has been reported for dipeptides composed of X-Ser or X-Gly. It is known that SDF-1 is digested by DPPIV/CD26 and lost binding activity to the CXCR4 receptor. In this study, we made a recombinant SDF-1 that has N-terminal extra three amino acids (Ser-Gly-Ser). After recombinant SDF-1 incubated with DPPIV/CD26, Digested SDF-1 protein activity was measured by chemotaxis cell migration assay. The chemotatic activity of digested SDF-1 interacting with the CXCR4 receptor is similar to recombinant SDF-1. It can be suggested that N-terminal extra Ser provides resistance to DPPIV/CD26 and maintains the proteins activity although recombinant SDF-1 was digested by DPPIV/CD26.

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Structural analysis and Functional study of Smr domain in Human B3bp

정의영, 송경미, 전위정, 이성환, 최성진, 조헌호, 반창일

포항공과대 화학과

The Small MutS-related domains (Smr domain), which are widely conserved from prokaryote to eukaryote, possess nicking endonuclease activity, incising the phosphate at the 3′ backbone position of DNA. Human Bcl-3 binding protein (B3bp) has a C-terminal Smr domain that functions as a nicking endonuclease. In order to verify the importance of N-terminal region connecting the Smr domain, we investigated the N-terminal extended Smr domain (exHSMRD; residues 1618-1770) and the Smr domain (HSMRD; residues 1691-1770) of B3bp through the use of a functional assay, SAXS (small-angle X-ray scattering analysis) and X-ray crystallography. The exHSMRD showed a random DNA endonucleolytic activity unlike the nicking endonuclease activity of the HSMRD. The low-resolution structure of the exHSMRD has been acquired by SAXS, and the crystal structure of the HSMRD was solved at 1.9 Å resolution with a crystallographic R-factor of 18.7%. We showed that the exHSMRD structure has an N-terminal elongated form rather than a globular HSMRD structure. Based on comparisons with other Smr structures, we might predict the amino acids that bind to DNA/RNA nucleotides. We suggest that the structural and functional differences between the nicking endonuclease HSMRD and the DNaseI-like endonuclease exHSMRD are affected by connecting the N-terminal region with the Smr domain.

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Purification of Importin alpha 3 for the studies on structure and function

최성진, 송경미, 전위정, 정의영, 이성환, 조헌호, 반창일

포항공과대 화학과

In eukaryote, importin alpha family binds with proteins containing nuclear localization signal (NLS) to move into nucleus through nuclear pore. Among the NLSs, classical NLS (cNLS) has been well studied. cNLS involves monoparite and biparite. Monoparite has one cluster of amino acid sequences and bipartite has two clusters of amino acid sequences. Recently novel cNLS has been revealed. Human importin alpha family is composed of importin alpha 1~7. Importin alpha family has high amino acid sequence identity but importin alpha family recognizes and specifically interacts with each NLS. To date, there were structures of human importin alpha 2, yeast importin alpha and mouse importin alpha 2 with their peptides containing NLS. In this study, we purified importin alpha 3 for study on structural analysis between importin alpha 3 and peptides containing NLS.

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Study on detection system for kanamycin using new aptamer by gold-nanoparticle colorimetry

송경미, 전위정, 정의영, 이성환, 최성진, 조헌호, 반창일

포항공과대 화학과

Kanamycin is an aminoglycoside antibiotic, used to treat a wide variety of infections. It induces mistranslation and blocks translocation by interaction with 30S subunit of prokaryotic ribosome. But, if it abuse to human through intake with food and over-prescription with medicine, it causes serious side effects include loss of hearing, toxicity to kidneys, and so on. So, it is important to use suitable amount and correct usage. Specially, plants and animals treated kanamycin for food have to check permissible level before sales and distribution. In this sense, aptamer against kanamycin which has potential as bio-probe and detection method using this are being researched. Aptamers are single strand DNA, RNA or peptide which have high affinity with target molecules. Here we report the ssDNA aptamer selected by SELEX using affinity chromatography. The binding affinity between ssDNA aptamer and kanamycin and binding region of ssDNA aptamer was confirmed by colorimetric method using goldnanoparticles. Based on these results, the selected ssDNA aptamer will be able to develop of biosensors for detection of kanamycin which is contained in food product.

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Small Angle X-ray Scattering Studies on Structures of Biological Macromolecules

진경식, *이문호

*포항공과대 포항가속기연구소 *포항공과대 화학과*

Individual molecules that actuate a specific response are thought of as the functional componentsof future nanodevices. Envisaged nanoassemblers and nanobots will require molecular-sized motors that can work efficiently in generating motion and forces. DNA is considered a versatile building block for such molecular machines because of its well defined structure and controllableintermolecular interactions. Several excellent reviews describe the application of DNA for the controlled self assembly of three-dimensional nanostructures, nanomechanical devices, and sensors. We are particularly interested in improving the usefulness of DNA nanomachines by improving their basic mechanical and switching functions and stability. Chemical functionalization of DNA can influence the inter- and intra-molecular bonds and, therefore, the stable molecular conformations. Controlled switching of the DNA between these states directly determines the mechanical force and displacement generated during the contraction/expansion cycle. Similarly, the stability of the different conformations will be determined by the free energy changes during switching, and highly stable states are desired for molecular logic. In this study we show for the first time that the attachment of fullerenes to a DNA motif significantly improves the molecular switching and stability of this pH driven enthalpic molecular machine.We are interested in developing biocompatible molecules with controllable, accurate and reproducible molecular motor functions. Our objective was to follow in detail the molecular conformation changes occurring in a DNA motif using three-dimensional molecular analysis by small angle x-ray scattering (SAXS)

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Synthesis of 3'-O-Allyl Fluorescent Nucleotides as a Reversible Terminator for Next Generation DNA Sequencing by Synthesis (SBS)

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*고려대 화학과 *KIST 생체과학연구부*

Next-Generation DNA Sequencing (NGS) opened DNA sequencing by synthesis (SBS) is one of the successful technology among Next-Generation DNA Sequencing (NGS). Current SBS technology is based on the CRT method, which is comprised of a three-step process of incorporating modified nucleotides, fluorescence imaging, and deprotecting for running the next cycle. This method requires dual-modified reversible terminators (DRTs), modified nucleotides having a reversible blocker on 3'-OH and fluorescent groups labeled on nucleobases for terminating DNA synthesis and for base-calling, respectively. In this regard, we designed and synthesized mono-modified reversible terminators (MRTs) in which the reversible blocking group on 3'-OH plays a role as a fluorescence-signal reporter as well as a reversible terminator. Allyl-based MRT linker was prepared from 1,5-pentanediol in ## steps, in which Fmoc protected amine group are adopted to introduce fluorophores. Alkylation of linker with 3'-OH of deoxyribose, and triphosphorylation gave new SBS sequencing probes with mono-modified reversible terminators, which were successfully incorporated by an engineered DNA polymerase.

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Apolipoprotein A-I mimic peptide with naphthyalanine can enhance cholesterol efflux from macrophage

김예원, *유재훈

*서울대 화학교육학과 *서울대 화학교육과*

Apolipoprotein A-I mimetic 4F (DWFKAFYDKVAEKFKEAF) is an amphipathic α-helical peptide with hydrophilic and hydrophobic spheres. Both faces of the peptide make intermolecular interactions with another molecule of the same peptide or with cholesterol/ester, forming high density lipoprotein-cholesterol (HDL-C). A variety of amphipathic peptides has been designed and synthesized as mimicry of 4F by substitution of the most important amino acids to unnatural amino acids both in hydrophilic and hydrophobic faces. These variants were screened for a mimicry of apoA-′ using HDL-C induced cholesterol efflux and tryptophan fluorescence intensity assays. A peptide (2S) with naphthylalanine moiety among these variants showed more than 3-fold improved cholesterol efflux than that of the reference peptide, 4F. Fluorescence intensity of 2S in the presence of liposomes showed specific interactions between cholesterol and naphthyl moiety in the peptide. Particles of cholesterol and the peptide were specifically uptaken by SRB1-rich CHO cells, suggesting that this peptide helps to clear out HDL-C-like particles in blood through hepatic cells. Taken together, new apo-AI mimetic peptides can be used as a potential therapeutic for releasing risks of atherosclerosis.

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Small α-helical peptides as inhibitors of anti-apoptotic Bcl-2 proteins

허연, 유재훈

서울대 화학교육과

Bcl-2 related proteins governs mitochondrial outer membrane permeabilization. Thus, they could be either pro-apoptotic or anti-apoptotic. We hypothesized that amphiphilic peptides with seven lysine and eight leucine residues and its derivatives can bind to Bcl-2 protein so that inhibit the release of cytochrome c into the cytosol, leading to apoptosis. We designed and synthesized a library of peptides with variations on hydrophilic face of the original peptide. Various natural and non-natural amino acids with carboxylic side chain were introduced to the helical peptide. Binding affinities of these resulting peptides against Bcl-2 were carried out, employing a florescence polarization competition assay. Among various α-helical peptides, we found out one peptide with dissociation constant in picomolar range against Bcl-2. This peptide not only gave a strong affinity but also showed an excellant selectivity that was proved by comparison with binding affinities against mutants of Bcl-2. In cell based assay, this peptide also showed strong apoptotic effect that was assayed by MTT and FACS analysis. This peptide, then, can be used as a potential therapeutic for treatment of cancer.

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A possible methylation-mediated control of Aurora kinase B phosphorylation activity uncovered with epigenetically modified histone H3 N-terminal peptides

한아름, 현순실, 유재훈

서울대 화학교육과

Epigenetic changes through post-translational modifications (PTM) are widely used to generate on/off switches for protein-protein interactions which serve as important gene controls in cells. N-terminal histone proteins have extensive epigenetically varied sequences, especially in H3. A variety of epigenetically modified peptides that mimic the H3 histone N-terminus were prepared and the AuroraB kinase catalytic efficiencies of these modified peptides were determined in this investigation. The data show that the peptide with mono-methylation at K4 (130%) has a higher activity toward the kinase. Other peptides with methylation modifications at K4 and K9 have slightly reduced kinase activities (20-80%). In contrast to those modified by methylation, peptides containing acetylation modifications have greatly reduced kinase activities (15%). Asymmetric and symmetric di-methylation at R2 and R8 leads to peptides that have low (9%) or non-existent activities, respectively. This observation supports the proposal that methylation and phosphorylation PTMs act as either cooperative (mono-methylation at K4) or reverse (di-methylation at R8) signal elements. It is clear that the results of in vitro kinetic studies using epigenetically modified histone H3 N-terminal peptide libraries can provide important information that leads to a greater understanding of the relationship between histone H3 N-terminal modification patterns and in vivo aurora B kinase activities.

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Selective α-glucosidase inhibitor elucidated by short aromatic peptidyl substrates

박상은, 현순실, 김희진, 유재훈

서울대 화학교육과

α-Glucosidases are one of the most abundant enzymes from a various sources from microorganism to more evolved animals and plants. These enzymes are essential for maintaining their catabolic metabolism, therefore, should be important targets if they are involved in pathogenicity. Many types of inhibitors, even commercially available drugs, for the target enzymes were discovered both from natural sources and synthetic sources. Some of them contain multiple carbohydrate rings and multiple hydroxyl groups. These inhibitors, therefore, aim carbohydrate binding sites of active site of the enzyme, affording usual nanomolar binding affinity. However, they generally lack specificity, affording side-effects by inhibiting other isozymes. Even though an inhibitor with a moderate affinity and good selectivity might be much more chance to become a drug candidate without side effects.In order to make specific inhibitor against this enzyme, we constructed a library construction of peptidyl-succinyl-α-D-glucopyranoside as substrates. Then, we selected the best substrate using chromogenic assay against various glucosidases. By carrying out this assay, we could elucidate complementary structure of the non-sugar part of the substrate pocket of the enzyme. The best substrate showed 50-fold improved Km value relative to p-nitorpheyl-α-D-glucopyranoside for the enzyme. Non-carbohydrate part of the substrate was a weak inhibitor against the cognate enzyme. In order to make this inhibitor stronger, this complementary structure was tethered to various general sugar moieties. Among them, β-glycosidic tethering molecule afforded Ki value in low micromolar ranges. Discrimination ratios of this inhibitor against cognate and other α-Glucosidases showed at least 10, suggesting that the peptydyl moiety is essential for the selectivity against glucosidase. This strategy can be generally applied for all inhibitors against a variety of pathogenic glycosidases.

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A Production of Specific MicroRNA Is Enhanced by Dicer Nuclease in the Presence of Trptophan-Containing Amphiphilic Peptides

한아름, 현순실, 유재훈

서울대 화학교육과

Drosha and Dicer are two key endonucleases for biogenesis of endogenous cis-acting microRNAs (miRNAs) that regulate target mRNA. Drosha converts pri-miRNA to ~ 70 nucleotide (nt) pre-miRNA in nucleus and Dicer converts pre-miRNA to linear ~22 nt single-stranded miRNAs in cytosol. We have synthesized Trp-containing amphiphilic peptides against several pre-miRNA targets. Peptide 2b showed a picomolar affinity and a keen specificity against pre-let7a-1 hairpin RNA. On treatment with this peptide, Dicer nuclease activity was selectively enhanced so that matured let7a-1 was produced more than reference samples. Northern blot experiment using human colon carcinoma also showed that specific increases of matured let7a-1 miRNA only in the presence of the specific peptide. As a result, non-specific Dicer nuclease is now converted to a specific therapeutic target by addition of the peptide that seems to change conformation of the pre-miRNA. While some exogenously delivered siRNA showed no sequence-specific effects as therapeutics, these kinds of hairpin-specific peptides can be alternative therapeutics to control endogenously derived miRNA.

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Detection of Human MC1R Gene Variant by DHPLC

김진호, 안영창, 조민호, 윤일규, 정덕현, 이은영, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Although human pigmentation is genetically complex, to date polymorphism at only 1 locus, the melanocortin-1 receptor (MC1-R), has been associated with physiologic variation in hair and skin color. The MC1-R, a G protein–coupled receptor with 7 transmembrane-spanning domains, plays a key role in determining the type of melanin (eumelanin vs pheomelanin) that is produced within melanocytes. Arg163Gln, a variant found infrequently in Europeans, was present in over 70% of East/Southeast Asians and Native Americans. Denaturing high performance liquid chromatography (DHPLC) is a relatively technique utilizing heteroduplex formation between wild-type and mutated DNA strands to confirm mutations and was predicted to be a potentially useful genotypic screening method for human MC1R gene variant. In this study, we need to test samples(KOREA populations) detection for human MC1R gene variant in hair follicle. We found that Arg163Gln variant occurs(happens) plentifully from a Koreans.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Confirmation of HER-2/neu Gene Overexpression from Breast Cancer Tissues

이은영, 안영창, 조민호, 윤일규, 정덕현, 김진호, *장원철

*단국대 화학과 *단국대 첨단과학대학*

HER-2/neu gene are located on chromosome 17 include tumour-suppressor genes P53 and BRCA1, and the gene for topoisomerase IIα. Numerical aberrations of chromosome 17 are linked to breast-cancer initiation and progression, and possibly to treatment response. The extent of amplification or protein overexpression typically is analyzed by fluorescence in situ hybridization (FISH) or immunohistochemistry (IHC), but quantitative PCR techniques have been described that may provide alternatives to these methods. The real-time PCR method offers several advantages. First, the real-time PCR method is performed in a closed-tube system and requires no post-PCR manipulation of sample. Second, this method supports the use of a normalization gene for quantitative PCR by fluorescent detection. Therefore, we confirmed of HER-2/neu gene overexpression from breast cancer tissues using real-time PCR quantification method. The HER-2/neu copy number was quantified in breast cancer tissues, as a result confirmed of different amplification signal curves.

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Detection of Lamivudine-Resistant Hepatitis B Virus by Fluorescence Probe

정덕현, 안영창, 조민호, 윤일규, 이은영, 김진호, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Hepatitis B virus (HBV) infection causes cirrhosis and hepatocellular carcinoma. Lamivudine (LAM) has been successfully used to treat HBV infections but prolonged use leads to the emergence of drug-resistant variants. Common diagnostic methods for mutation such as sequencing and restriction fragment length polymorphism (RFLP) analysis lack sensitivity and require significant processing. Thus, a rapid and accurate diagnosis is important the lamivudine-resistance mutation. In this study, lamivudine-resistance mutation is detected by fluorescence probe with Real-time PCR in HBV patients. The results of the real-time PCR assay were consistent with the DNA sequencing. As a rapid, accurate method, real-time PCR assay should be useful for detecting lamivudine resistance variants during lamivudine therapy in clinical settings.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Isolation of c-reactive protein from human serum using phosphocholine coated magnetic nanoparticles

김은주, 김현철, 정상원

대구경북과학기술원 나노바이오연구부

Phosphocholine coated magnetic nanoparticle was synthesized to isolate c-reactive protein from human serum. CRP is one of the pentraxin proteins and has five calcium-dependent binding sites for phosphocholine. Methacryloxypropyltrimethoxysilane (MPS) coated magnetic nanoparticle was synthesized (~15 nm) and a phosphocholine-containing monomer (12-(4-vinylbenzyloxycarbonyl)dodecyl phosphocholine, VPC) was synthesized by sequential introduction of 4-vinylbenzyl and phosphorylcholine groups into 12-hydroxyldodecanoic acid. The VPC was polymerized to MPC coated MNP by addition of AIBN and stirred for 2 hrs at 70℃. The CRP was isolated by VPC coated MNP from human serum, and the binding capability was analyzed by ELISA and SDS-PAGE. The surface modification was confirmed by FTIR and XRF analysis.

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Expression and purification of goldfish Cytochrome p450 1A by using yeast system

CHANG ZIWEI

부산대 화학과

Cytochrome P450 1A (CYP1A) is the most important gene family involved in the metabolism of xenobiotics and elevated expression of cytochrome P4501A (CYP1A) is an established biomarker for exposition to a wide range of toxicants, particularly for dioxin and structurally similar compounds. As the cDNA of goldfish CYP 1A has been cloned, here we expressed and purified CYP 1A using a yeast system. Goldfish CYP1A gene was ligated into expression vector pREP42-mhn to generate the recombinant pREP42-MHN-CYP plasmid. The vector was transformed into Yeast strain Schizosaccharomyces pombe ED665. The protein was purified by Nickel column and checked by SDS-PAGE.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Effects of human heat shock transcription factor 1 on mouse embryonic fibroblasts cells

박성민

부산대 화학과

Under various stress conditions such as heat, UV, and chemical reagents, heat shock transcription factor 1(HSF1) plays important roles in heat shock protein expression. In previous study, it was found that some amino acid residues in human heat shock transcription factor 1(hHSF1) are essential to activate hHSF1 in *in vitro* experiments. Here, we found that wild type and some mutants of hHSF1 affect cell survival under circumstances of heat stress. Vectors containing hHSF1 genes were transfected to mouse embryonic fibroblasts (mEF) and the level of heat shock proteins after heat shock were detected by western blot.

한국화학회 KOREAN CHEMICAL SOCIETY

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PH Effect on Iron Autoxidation and Fenton-type Oxidation

김영란, *노상균, 김종문, 김석규

*영남대 화학과 *동양대 화학공학과*

Iron is indispensable element in cell metabolism. However, free iron ions are apt to be oxidized to generate highly reactive oxygen species (ROS), including superoxide radical ($O_2^{\bullet-}$) and hydroxyl radical ($OH^{\bullet}$), resulting in the modification or destruction of cellular molecules, such as DNA, protein, and membrane, etc. There are two well-known mechanisms illustrating the iron-mediated ROS generation process. One is Fenton mechanism in which Fe^{2+} reacts with endogenous H_2O_2 to produce hydroxyl radicals. The other is iron-autoxidation with the reaction of molecular oxygen. These two mechanisms seem slightly different in their efficiencies and kinetics in the DNA cleavage, hydroxyl radical generation, and the oxidation of Fe^{2+} to Fe^{3+}. In both cases, it is obvious that chelating agents, such as phosphate and citrate, are prerequisite. In order to elucidate the difference between these two mechanisms, we compared the pH effect on the iron oxidation, hydroxyl radical generation, and DNA cleavage reaction.

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Molecular Cloning and Protein Overexpression of Goldfish hsp70, and Its Applications for Monitoring the Environmental contamination

배민지

부산대 화학과

HSP is included in Molecular chaperones. Molecular chaperones are major cell constituents in all organisms under nonstress conditions and they are essential to ensure proper folding and intracellular localization of newly synthesized polypeptides. 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. We obtained the full-length hsp70 c DNA from goldfish liver, and cloned it into pQE30 vector. After overexpression and purification, hsp70 proteins were injected into mouse for making anti-hsp70 antibody.Here, then hsp70 antibody could be used to monitoring the environmental pollution.

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Conformational Studies of the Mimotope Peptide of Apolipoprotein B4i by NMR Spectroscopy

Khan asghar, 원호식

한양대 응용화학과

Apolipoproteins are protein components of lipoproteins exhibiting major roles in the transport of plasma lipids and used clinically for the of coronary artery disease. A number of mimetic peptides of apolipoproteins were screened from the phage-displayed random peptide library by using a biopanning method. The mimetic peptides were recognized by the monoclonal antibody against apo B-100 specific monoclonal antibody was $(CRNVPPIFNDVYWIAF)_4$(B4i). Theses amino acid sequences of peptides are not in original antigens apo B-100. Compared with primary arrangement of amino acid using of BLAST search B4i were confirmed 40% homology with apo B-100. In this study, ^{1}H-NMR and 2D NMR(COSY, TOCSY, NOESY) experiments were accomplished and signal assignments of mimotope peptides were made. Distance of numerous proton paris were obtained based on the NOE cross peak intensities of NOESY spectrum. On the basis of these distance data, distance geometry(DG) and molecular dynamic(MD) were carried out to determine the tertiary structure of mimotope B4i. DG structures of three mimotope B4i were low penalty value 0.3~0.6 $Å^2$, and the total RMSD obtained upon superposition of all atoms were in the range 0.5~1.5Å. Mimotope B4i has a similar 3_{10}-helix structure from Ile^7 to Trp^{13}

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Structural Study SM(E122K) by NMR Spectroscopy

김연주, 원호식, 최현주, 우선희

한양대 응용화학과

Adenylate kinase from Mycobacteria tuberculosis (AKmt) is an essential enzyme for the survival of the microorganism. This enzyme is highly homologous in its amino acid sequence with mammalian AK1. In spite of the structural homology, the enzyme activity of AKmt is poor one fourth from the AK1. The purpose of the present study was to restore the enzyme activity of AKmt to the same level as AK1 on the basis of structure-function relationship. AK family has three domains; AMP binding domain (AMPbd), ATP binding domain(ATPbd), and the 122nd glutamate at analogically LID domain, For protein engineering, the 122nd glutamate with lysine(E122K). Replacements were made with the corresponding amino acid residues of AK1. I constructed one point-mutant(E122K) rspectively. As results, the point mutant showed a little enhanced catalytic activities.In order to identify the role of substitution of Lys[122], 3D-NMR experiments including 15N-HSQC, show that ATP binding P-loop(7-13) and LID domain and include LID domain surrounding residues(115~135), are slightly perturbed($\delta w \approx 0.1$~03ppm) and 1H-13C-15N correlated NOESY for structure determination have been carried out. NMR-based solution-state structures of AKmt and Lys[122] are in progress with NOESY data. On the basis of AKmt and previous results, we propose that it looking to structurally changed K122 and R1, R2 values are calculated through T1/T2 and titration experiment, this value is to investigate the characteristics of the E122K. As a results, More flexible dynamic motion of LID domain and electrostatic interactions of LID and Core domain of AKmtSM will be able to contribute to catalytic activity enhancement and overall stability

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NMR study for the B-Z transition of DNA duplexes induced by the Z-DNA binding protein

이은해, 이준화

경상대 화학과

The Z-DNA binding protein (Zα) binds tightly and specifically to left-handed Z-DNA. This protein has subsequently been found in the vertebrate RNA editing enzyme double-stranded RNA adenosine deaminase1 (ADAR1), mammalian protein DAI and E3L virulence factor of poxviruses. The co-crystal structure of Zα protein complexed to Z-DNA showed that one monomeric Zα protein binds to one strand of double-stranded DNA and a second Zα protein monomer binds to the opposite strand with the 2-fold symmetry with respect to DNA helical axis. It remains unclear how Zα protein specifically recognizes Z-DNA sequence in a sea of B-DNA to produce the stable Zα-Z-DNA complex during the B-Z transition induced by Zα protein. In order to investigate the sequence effect on the DNA binding affinity and B-Z conversion activity of various Zα proteins, we performed NMR experiments with complexes of Zα proteins bound to DNA duplexes produced at a variety of protein-to-DNA (P/N) molar ratios. Comparison of these results suggests that Zα proteins binds to Z-DNA via an active B-Z transition mechanism, where Zα exhibits the sequence preference of d(CGCGCG)2 >> d(CACGTG)2 > d(CGTACG)2 through multiple sequence discrimination steps.

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Cracked Iron Oxide Nanoparticles for MR Imaging and Drug Delivery

채민경, *이철현, **조지현, **황정순, *장은주

*한국기초과학지원연구원 *한국기초과학지원연구원 자기공명영상팀 **한국기초과학지원연구원 자기공명연구부*

Magnetic nanoparticles have a unique properties and abilities to do molecular imaging and biomedical applications. Iron oxide nanoparticles are usually safer than other potentially toxic metal ions such as Gd3+ and Mn2+ in the body. Furthermore, hollow sphere iron oxide nanoparticles have a good r2 relaxivities and space to fill therapeutic agents. Accordingly, we synthesized nontoxic cracked iron oxide nanoparticles (CION) from hydrophobic FeO nanoparticles (HION) via 3 steps. It showed improved r2 relaxivities and potential application as a drug delivery system. It will be discussed to examine the drug delivery potential for CION loaded with DOX and its evaluation of cellular uptake by using HT-29, a human tumor cell.

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Hydrogen exchange study of Z-DNA complexed with the Zβ domains of DAI protein

김희은, 이준화

경상대 화학과

Left-handed Z-DNA is high energy conformation than right-handed B-DNA and forms in a polymer of alternating pyrimidine-purine sequences. Z-DNA is stabilized by negative supercoiling generated during transcription or by complex formation with the Z-DNA binding proteins in vivo. Double-stranded RNA deaminase I (ADAR1) has two left-handed Z-DNA binding domains, Zα and Zβ, at its NH2-terminus. The Zα domain of human ADAR1 (ZαADAR1) preferentially binds Z-DNA rather than B-DNA with high binding affinity. The crystal structure of the ZαADAR1′ Z-DNA complex revealed that the monomeric Zα domain binds to one strand of Z- DNA, while a second monomer binds to the opposite strand, yielding twofold symmetry with respect to the helical axis. Human DNA-dependent activator protein of IFN-regulatory factors (DAI) is central to activator of the innate immune response. Human DAI binds left handed Z-form DNA with high affinity and it shares similar DNA-binding domains (Zα and Zβ) to the vertebrates ADAR1. The crystal structure of the ZβDAI-Z-DNA complex reveals that ZβDAI has a similar fold to that of other Z-DNA binding Domains, but adopts an unusual binding mode for recognition of Z-DNA. In order to characterize the molecular recognition of Z-DNA by ZβDAI and compare with that of hZαADAR1, we performed NMR experiments on complexes between the ZβDAI and DNA duplexes with a variety of protein-to-DNA molar ratios. These results provide insight into the unique B-Z transition mechanism induced by ZβDAI.

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ENZYMATIC INCORPORATION OF 3'-O-FLUORESCENTLY MODIFIED NUCLEOTIDES FOR SEQUENCING-BY-SYNTHESIS

김다래, *권혁성, **안대로, ***신동윤

*고려대 생명공학과 *KIST 의과학센터 **KIST 생체과학부 ***KIST 생체과학연구부*

Incorporation of 3'-O-fluorescently modified nucleotides by a DNA polymerase was examined. Due to the blocking groups on the 3'-OH, termination of DNA synthesis was observed after extension of a single nucleotide in the primer. Since the linker is chemically cleavable under DNA compatible conditions, those modified nucleotides may further be used as reversible terminators in sequencing-by-synthesis (SBS)

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Real-time PCR based on fluorescence polarization

송하은, *최연경, **안대로, ***김다래

*동덕여대 응용화학과 *KIST 의과학센터 **KIST 생체과학부 ***고려대 생명공학과*

Real-time PCR is one of most popular methods for quantitative analysis of genes found in various research fields. Currently, DNA binding dyes and oligonucleotide-based molecular beacons are being used to lively report the amplification process with fluorescence signal. Here, we present a novel real-time PCR method which utilizes fluorescence polarization to monitor PCR amplification.

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Investigation on the roles of catalytic residues of Scp1 in its catalytic mechanism

김영준

건국대 응용생화학과

Human small C-terminal domain phsphatase 1 (Scp1) modulates the phosphorylation state of the C-terminal domain (CTD) of eukaryotic RNA polymerase II (RNAP II), with preference for phosphorylated Ser5 in the tandem heptad repeats of CTD (Y1-S2-P3-T4-S5-P6-S7). Additionally, Scp1 was identified as a conserved regulator of neuronal stem cell development. Scp1 is a member of haloacid dehalogenase (HAD) superfamily, whose catalysis depends on a Mg ion and a DXDX(T/V) motif. The first Asp of the motif is identified as the nucleophile that is subject to phosphorylation leading to a phosphoryl-aspartate intermediate. This high-energy mixed anhydride intermediate is subsequently hydrolyzed to regenerate the enzyme. Scp1 has several residues for its catalytic activity, such as D96, D98 and D206. According to recently Scp1 study, it follows double general acids mechanism instead of general acid and base mechanism. Therefore, we would like to confirm this mechanism through kinetic and structural investigation with certain mutants of Scp1.

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Environmental pollution research of marine mussels (Mytilus edulis) using NMR metabolomics

박종철

한국기초과학지원연구원 분석연구부

Marine mussels (Mytilus edulis) have been widely used as biomonitors because they can be subjected to environmental stresses and pollutants in the natural environment. In this study Mytilus edulis was aimed at investigating the metabolic pathway on the heavy metals. Extracts of mantle tissue from mussels were analyzed by using 1H-NMR spectroscopy to provide metabolic fingerprints associated with these heavy metals. Moreover heavy metal concentrations were analyzed by using ICP-MS. Discriminant analysis showed significant metabolic differences between mussels from environmentally polluted and normal areas which are indicated by a clear separation into two groups. Mussels from polluted area were associated with an increase in the concentration of arginine, betain, creatine, leucine, methionine, serine, succinate and threonine, and a decrease in the concentration of choline (P

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Bioinformatic prediction of Drosophila melanogaster phosphatome

권우중, Mrigendra B. Karmacharya, 소재원

인하대 화학과

A phosphatase is an enzyme that removes a phosphate group from its substrate by hydrolysing phosphoric acid monoesters into a phosphate ion and a molecule with a free hydroxyl group. This action is directly opposite to that of phosphorylases and kinases, which attach phosphate groups to their substrates by using energetic molecules like ATP. Approximately 30% of cellular proteins have been shown to contain covalently bound phosphate. 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. Protein phosphatases are amongst the extensively studied proteins and are reported as potential drug targets of many diseases including cancer and others. Here, we identified, classified, and analyzed protein phosphatases in fruitfly. We report at least 70 putative protein phosphatases in fruitfly which include 27 PSTPs, 33 PTPs and 10 Asp-based protein phosphatases. We modeled 3D structures of the catalytic domains of these putative protein phosphatases.

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Novel roles of PKG isoforms in cyclin D1 transcription

rana md sohel, 소재원

인하대 화학과

Although protein kinase G (PKG) plays important role in the inhibition of cell proliferation and cell cycle progression, the isoform-specific role of PKG in mediating these functions is still obscure. To elucidate the role of PKG isoforms in transcriptional control of cyclin D1, we employed a series of expression vectors of PKG 1α and PKG 1β which encode hemagglutinin-tagged wild type (WT) and constitutively active (SD and ΔN) mutants. In our present study we found that both the constitutively active mutants of PKG1β downregulate the transcription of cyclin D1 when transiently transfected in NIH3T3 cells, whereas PKG 1α mutants show weak inhibition. We further studied the transcriptional regulators of cyclin D1, such as, c-fos, NF-κB, and CRE by using the luciferase reporter assay. Constitutively active mutants of PKG 1β showed better transcriptional downregulation of c-fos in NIH3T3 cells, whereas PKG 1α downregulated c-fos to a lesser extent. We also found that the constitutively active mutants of PKG negatively regulate the activation of NF-κB and CRE, suggesting their involvement in the regulation of cyclin D1. Thus we can conclude that PKG activation downregulate the transcription of cyclin D1 in NIH3T3 cells.

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Comparative analysis of protein phosphatases in Arabidopsis genome

Mrigendra B. Karmacharya, 소재원

인하대 화학과

Reversible phosphorylation is a critically important step in the functional regulation of a protein. 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 many 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. Here, we identified at least 142 putative protein phosphatases in Arabidopsis genome. We classified these proteins into five groups on the basis of the catalytic protein phosphatase domains present on them. We analyzed the expression profiles of each Arabidopsis phosphatases. We modeled three dimensional structures of these proteins. We performed in silico docking of Arabidopsis PP2A with okadaic acid and calculated the affinity energy (-10.9kcal/mol) between them. Furthermore, we extended our study in rice genome to find out the Arabidopsis protein phosphatase orthologs in rice.

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Design and Synthesis of 1-Phenyl Barbituric Acid Containing N-Substituted Indole Derivatives as a Non-Competitive Inhibitor against PTP1B Enzyme

khadka deegendra, Kafle Bhooshan, Aher Nilkanth G., 조형진

인하대 화학과

As most intracellular signaling takes place via cascades of phosphorylation and dephosphorylation of tyrosine, protein tyrosine phosphatases have emerged as new and promising target for type 2 diabetes and obesity. Among them, protein tyrosine phosphatase 1B (PTP1B) negatively regulates insulin signaling by dephosphorylation, thereby attenuating receptor tyrosine kinase activity. Thus, PTP1B inhibitor could potentially ameliorate insulin resistance. So, we have synthesized 1-Phenyl barbituric acid containing N-substituted indole derivatives as PTP1B inhibitor and their enzyme assay experiments were performed. Most of the analogues had potencies in low micro molar ranges. Enzyme kinetics studies revealed thatthe compound inhibits PTP1B was a reversible non-competitive inhibitor.

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Design and Synthesis of 5-Arylidene-2-arylimino-4-thiazolidinones as PTP1B inhibitors

Aher Nilkanth G., Kafle Bhooshan, khadka deegendra, 조형진

인하대 화학과

Protein tyrosine phosphatase 1B (PTP1B) is an effective target for the treatment of both type 2 diabetes and obesity; however, targeting PTP1B for drug discovery is challenging because of the highly conserved and positively charged active-site pocket. Tremendous progress has been made in the development of potent and selective PTP1B inhibitors. As part of a project aimed at identifying effective nonphosphorus monoanionic inhibitors of PTPs, we have synthesised a series of novel 2-amino-5-alkylidene-thiazol-4-ones, and their activities as inhibitors of PTP1B were evaluated. All the compounds showed inhibitory potencies, some of the compounds showed interesting inhibition levels in the low micromolar range (IC50 = 5 – 0.98 μM). The 5-arylidene moiety of acids proved to markedly influence the potency of these inhibitors.

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Production and Structural Characterization of Antibacterial Peptide, LPcin

김지선, 박태준, 김용애

한국외국어대 화학과

Lactophoricin (LPcin-I) is a cationic amphipathic peptide with 23 amino acid residues, and corresponds to the carboxy terminal 113 to 135 region of PP3. LPcin-I inhibits the growth of both gram-negative and gram-positive bacteria, but has no hemolytic activity at concentrations of less than 200mM. In contrast to LPcin-I, it has been reported that LPcin-II, which corresponds to the 119 to 135 region of PP3, has no antibacterial activity, which is interesting because LPcin-I and LPcin-II have similar charge ratios and identical hydrophobic/hydrophilic sectors based on the helical wheel pattern. Furthermore, both peptides show cationic and interact with phospholipids. Nevertheless, only LPcin-I is incorporated into planar lipidic bilayers, in which it forms voltage-dependent channels. In order to understand the antibacterial mechanism of LPcin-I and structure-activity relationships between LPcin-I and LPcin-II, we cloned and expressed two recombinant peptides in the form of inclusion bodies as a ketosteroid isomerase (KSI) fusion proteins in Escherichia coli. Fusion proteins were purified by IMAC under denaturing conditions, and cleaved from fusion by CNBr. Final purifications were achieved by preparative RP-HPLC. We obtained more than ten milligrams of N^{15} labeled peptides per liter of growth, which was sufficient for solid-state NMR spectroscopy. Structural characterizations in the membrane-like environments were obtained by circular dichroism, solution and solid-state NMR spectroscopy. Peptide engineering and structural characterization were done to search for the shortest antimicrobial peptide.

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Inhibitory effect of eugenol with antioxidant activity on MMP-2 and MMP–9 related to metastasis

남향, *김문무

*동의대 화학과 *동의대 자연대학/화학과*

The oxidative damage of lipid, protein and DNA is known to be involved in chronic inflammation such as arthritis, hepatitis, nephritis, gastritis, colitis and periodontitis. It has been highlighted for searching natural compounds without toxicity which prevent development of these diseases. Thus, we studied whether eugenol(4-allyl-2-methoxy-phenol) can inhibit MMP expression and activity as well as antioxidant effect. Eugenol was contained as a major ingredient of herbs such as clove and *Magnoliae Flos*. The direct scavenging effects of eugenol on DPPH radical, hydrogen peroxide, lipid peroxidations and genomic DNA damage related to oxidative stress were evaluated *in vitro*. It was observed that eugenol exhibited higher inhibitory effect on hydrogen peroxide than other reactive oxygen species, and also blocked DNA oxidation and lipid peroxidation induced by hydroxyl radical. In addition, its inhibitory effects on the activity and expression of MMP-9 activity related to metastasis were determined using gelatin zymography and western blot. The data showed that it inhibited MMP-2 and -9 activities in PMA-stimulated HT1080 cells. Furthermore, It was found that eugenol exerts inhibitory effects on MMP-9 via inhibition of p-JNK and p-ERK. Therefore, these results suggest that eugenol could be available as an excellent agent for prevention of metasasis related to oxidative stress.

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Multiplex oligonucleotide-linked immunosorbent assay for the simultaneous detection of cancer markers

안대로, *한기철

*KIST 생체과학부 *KIST 의과학연구센터*

Early detection of cancer biomarkers provides clinically valuable information. While the conventional enzyme-linked immunosorbent assay (ELISA) has been routinely used for individual cancer markers, methods for simultaneous determination of multiple markers within a single sample are still in demand. Here, we present a novel oligonucleotide-linked immunosorbent assay (OLISA) with a multiplexing capability on the same microwell plate-based system as in ELISA. Employing a DNA oligonucleotide that is covalently conjugated to the detection antibody and a complementary RNA oligonucleotide which is appended with a fluorophore and a quencher, degradation of the RNA in the DNA-RNA duplex by RNase H is exploited for fluorescent signal generation. Iterative cycles of DNA-RNA duplexation and subsequent degradation of the RNA in the duplex by RNase H further lead to amplification of the detection signal in OLISA. Moreover, the unique nature of the signal amplification enables multiplexing of OLISA, which is successfully demonstrated by tethering DNA molecules to detection antibodies and by performing assays for three common cancer markers including alpha-fetoprotein, prostate specific antigen and carcinoembryonic antigen. With the simple procedure and reliable detection performance, the developed multiplex OLISA has a wide potential to be used for analysis of a panel of biomarkers in clinical diagnostics.

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Inhibitory effect of fucoidan on ROS induced oxidative damage and MMP-9 in HT1080 cells

권은정, 박인환, *김문무

*동의대 화학과 *동의대 자연대학/화학과*

Fucoidan(FCD) is a sulfated polysacacharide found mainly in various species of brown seaweed such as kombu, limu moui, bladderwark, wakame and mozuku. Especially enzyme-digested fucoidan extract has attracted a lot attention due to its anti-tumor potential. In this study it was observed that FCD exhibited the highest inhibitory effect on DPPH and hydrogen radical, and blocked DNA oxidation induced by hydroxyl radical. Furthermore, its inhibitory effect of FCD on MMPs expression was determined by gelatin zymography and western blot analysis. The inhibitory effect of FCD at 1 μg/ml on activity of matrix metalloproteinases -9 (MMP-9) was increased in human firosarcoma cells (HT1080). Moreover it specifically inhibited both activity and expression of MMP-9 via inhibition of ERK, a MAPK. In addition the expression level of MMP-9 gene was decreased in the presence of FCD. Theses result provide a evidence that FCD could be a potential candidate for cancer chemoprevention.

key word : HT1080, Fucoidan, Antioxidant, ERK, MMP-9

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Different Synthetic Method Lead to Different Toxic Effect in nano-sized ZnO

이상원, 박수진, 정민숙, 송미령, 김진현, 김준성, *이진규, *정학성, *임주현, **조명행

*(주)바이테리얼즈 부설연구소 *서울대 화학부 **서울대 수의과대학*

The aim of this study is to assess the toxicity and the physico-chemical characteristics of nano-sized ZnO. The single-phased ZnO were synthesized at two temperatures (RT and 60 ℃), which mainly affected particle sizes and the shape. ZnO-60 with a larger particle size (length; 80.5 ± 6.8 nm) is more toxic due to ROS in the MTT and a H2DCF-DA assay including an antioxidant (NAC) treatment. In ESR analyses employing spin-trap agents (DMPO and TEMP), signals corresponding to the hydroxyl radical (•OH) and the singlet oxygen (1O2) were detected, but they were reduced after treating scavengers (DMSO and NaN3). It is accordingly considered that the toxicity of ZnO is mainly caused by •OH and 1O2, and the toxicity due to ROS was dominant in larger particles synthesized with the heating process. Additionally considering ICP-AES analyses, the toxicity by Zn2+ ion might be a little in our study.

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NEW QUINONE DERIVATIVES FROM THE MARINE-DERIVED FUNGUS PHOMA SP

nenkep viviane nadeg, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

Marine-derived microorganisms continue to attract attention as a rich source of structurally novel bioactive metabolites that are potential lead compounds for the development of new drugs. As part of an ongoing search for new bioactive metabolites from marine-derived fungus, a marine alga-associated fungus, Phoma sp., was studied because the broth extract showed potent radical scavenging activity. An assay-guided purification resulted in isolation of two new radical scavenging quinine derivatives. We report here on the isolation, structural elucidation, and radical scavenging activity of new quinones.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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A BENZODIAZEPINE ALKALOID FROM THE MARIEN ALGAE-ASSOCIATED FUNGUS EXOPHIALA

Leutou Alain Simplic, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

Marine-derived microorganisms such as bacteria and fungi have proven to be a rich source of new biologically active secondary metabolites. As a part of our search for bioactive substances from the marine-derived microorganism, the marine alga-associated fungus was studied because the mycelium extract showed potent ultrviolet-A protecting activity. An assay-guided purification resulted in the isolation of an alkaloid, circumdatin A from the marine isolate of fungus Exophiala sp. We report here on the isolation and structural elucidation of the compound as well as the UV-A protecting activity.

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MICROBIAL TRANSFORMATION OF MELLEIN BY A MARINE-DERIVED BACTERIUM

fengzhile, *윤금자, *손병화, **최홍대

*부경대 화학과 *부경대 화학과 **동의대 화학과*

As part of a program to produce new compounds by the microbial transformation of the bioactive metabolites produced by fungi isolated from marine habitats, the microbial transformation of mellein was performed by a marine-derived bacterium using a two-stage culture protocol. After culture of Stappia sp. with mellein for 72 h, the culture broth was harvested, filtered, and extracted with EtOAc to yield the crude extract. The extract was purified by repeated Si gel flash chromatography (n-hexane in ethyl acetate) to yield the oxidized metabolite. Here, we will describe the isolation, structural elucidation, and the biological actives of the new metabolite.

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Development of an advanced PET/MRI nanoprobe with enhanced NIR fluorescence by dye encapsulation, and its application to deep tissue imaging

김진현, 김준성, 송미령, 정민숙, 박수진, 이상원

(주)바이테리얼즈 부설연구소

Noninvasive imaging technique is essential for the diagnosis and monitoring in biomedical application. But each of single imaging techniques has limitations. Therefore, the combination of these techniques was necessary to complement the limitations. In this report, we developed radiolabeled NIR-fluorescent magnetic silica nanoparticles, 68Ga-(MNP-SiO2(NIR797)) for PET/MR/NIRF images. This advanced nanoprobe shows strong contrast effect for PET/MR/NIRF images, biocompatibility for biomedical application, and the enhancement of the fluorescent intensity and stability compared to the free dyes. We also demonstrated our probe's contrast effect in vivo through sentinel lymph node (SLN) mapping by using PET/MR/NIRF images. Moreover, to evaluate the enhanced NIRF property by encapsulation of NIR fluorescent dye in the silica shell, we applied our probe for cell trafficking in the deep tissue (brain, spinal cord and liver). We injected cells labeled our probe into the deep tissue and then we obtained well distinguished NIRF images in the injected area. In conclusion, we developed radiolabeled magnetic silica nanoparticles that encapsulate NIRF dye in the silica to decrease toxicity, enhance the fluorescence stability and deep tissue imaging. We anticipate that this advanced probe provided a complementary role in imaging diagnostics and cell trafficking.

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Preparation of fluorescent polymer based silica core-shell nanoparticles for biological analysis

이창수, *장희현

*한국생명공학연구원 바이오나노연구단 *한국생명공학연구원 바이오나노연구센터*

Progress in biomedical imaging depends on the development of probes that combine low toxicity with high sensitivity, resolution, and stability. A new class of highly fluorescent core-shell nanoparticles with narrow size distributions and enhanced photostability, known as poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene (MEH-PPV) cores coated by silica-based shells were prepared with a reverse micelle method and their fluorescent properties. The morphologies, particle size distribution and fluorescent properties of MEH-PPV/SiO2 particles were characterized by transmission electron microscopy (TEM), scanning electron microscope (SEM), particle size analyzer and fluorescence emission spectra by DLS, UV, PL, ELS, confocal microscopy.

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Cloning of partial cDNA sequences encoding for relaxing peptide purified from starfish, *Asterina pectinifera*

고혜진, 조은희, 김혜림, 우경은, 서정길, 박남규

부경대 생물공학과

A peptide with a relaxing effect on the dorsal retractor muscle (DRM) was isolated from the starfish, *Asterina pectinifera*. The sequence of the purified peptide was analyzed by an automated amino acid sequencing and MALDI-TOF mass spectrophotometry. Molecular ion peak in the MALDI-TOF mass spectrum of the peptide was displayed m/z 1602 (M+H)+. The sequence of the peptide was determined to be FGKGGAYDPLSAGFTD. We determined the partial cDNA sequence of this peptide by degenerate polymerase chain reaction using the information of amino acid sequence. This partial sequence contained 483bp including 3' untranslational region 199bp.Based on the result of purification and cDNA works, this peptide turned out to have 16 amino acid residues. A database search indicated that this peptide similar to pedal peptide from California purple sea urchin, Strongylocentrotus purpuratus.

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Cloning of partial cDNA sequences encoding for SF-CNP with relaxing activity on the DRM purified from starfish, *Asterina pectinifera*

고혜진, 조은희, 김혜림, 우경은, 서정길, 박남규

부경대 생물공학과

The C-type Natriuretic Peptide-like peptide (SF-CNP) with relaxing activity was isolated from the whole body extract of starfish, *Asterina pectinifera*, using the dorsal retractor muscle (DRM) of the starfish as the bioassay system. The sequence of the purified peptide was analyzed by an automated amino acid sequencing and MALDI-TOF mass spectrophotometry. Molecular ion peak in the MALDI-TOF mass spectrum of the peptide was displayed m/z 2306.95 (M+H)+. We determined the partial cDNA sequence of this peptide by degenerate polymerase chain reaction using the information of amino acid sequence. This partial sequence contained 277bp including 3'untranslational region 202bp.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **BIO.P-57**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Cloning of partial cDNA sequences encoding for SF-CT with relaxing activity on the DRM purified from the starfish, *Asterina pectinifera*

고혜진

부경대 생물공학과

The calcitonin-like peptide (SF-CT) with relaxing activity was isolated from the whole body extract of starfish, *Asterina pectinifera* using the dorsal retractor muscle (DRM) of the starfish as the bioassay system. The SF-calcitonin was purified by ion-exchange and C18 reversed-phased HPLC. The primary structure was determined by a combination of an automated amino acid sequencing and MALDI-TOF mass spectra. Molecular ion peak in the MALDI-TOF mass spectrum of the peptide was displayed m/z 3655 (M+H)+. We determined the partial cDNA sequence of this peptide by degenerate polymerase chain reaction using the information of amino acid sequence. This partial sequence contained 569bp including 3'untranslational region 446bp.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **BIO.P-58**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Discovery and investigation of DNT-specific peptide

장현준, 이광규, 나정현, 이원규, 유연규

국민대 생명나노화학과

Biomolecules specific to explosives can be exploited as chemical sensors. Peptides specific immobilized dinitrotoluene (DNT) were identified using phage displayed library. A derivative of DNT that contained an extended amine group, 4-(2,4-dinitrophenyl)butan-1-amine, was synthesized and immobilized on self-assembled monolayer of gold surface. Peptide displayed M13 phages specific to the immobilized DNT-derivate were isolated from the M13 phage library displaying random sequence of 12-mer peptides by biopanning procedure. A phage displaying a unique 12-mer peptide sequence was amplified during biopanning process. A synthetic peptide was prepared and examined its binding affinity to DNT using isothermal titration calorimetry and surface plasmon resonance analysis.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-1**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Properties of π-Extended, Expanded Porphyrins: Rosarin, Rubyrin and Pyrrole-Inverted Sapphyrin

이창희, 유수연, *J. L. Sessler, *Jung-Su Park

*강원대 화학과 *University of Texas at Austin*

Several new pi-extended, expanded porphyrinoid macrocycles including naphthorosarin, naphthorubyrin and naphthosapphyrin were synthesized and fully characterized. The solid state structure of the naphthorosarin and naphthorubyrin were determined by single crystal X-ray diffraction analysis. The naphthorosarin exhibited unique spectroscopic properties, corresponding to those of antiaromatic compound in spite of planar geometry and global conjugation of double bonds. The most prominent feature in proton NMR spectrum is that the chemical shifts of the three core pyrrole N-Hs appear at 26.2 ppm, which is typical for the indication of anti-aromatic character. Naphthorosarin becomes paramagnetic and ESR active upon multiple protonation. The naphthorasarin was easily reduced upon treatment with sodium borohydride and the reduced compound becomes aromatic. Naphthorubyrin, on the other hand, shows typical aromatic characteristics. The compound was quite basic as other expanded porphyrins and mono-protonated form was isolated on regular work-up. The compound displayed large hypsochromic shift of Q-bands upon protonation/deprotonation process.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-2**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Calix[4]pyrrole-Crown-n (n=5,6) Ion-Pair Shopping-Baskets Displaying Anion-Modulated, Cation-Selective Binding and Transport

이창희, 김보향, 이유림, *J. L. Sessler, *Sung Kuk Kim

*강원대 화학과 *University of Texas at Austin*

Ditopic ion pair receptors, bearing tunable cation- and anion-binding sites, have been synthesized and characterized. Spectroscopic analyses confirm that the synthesized receptors bind with fluoride and chloride anion strongly and both form stable 1:1 complex in acetonitrile. When the corresponding anion complexes were treated with alkaline metal ions (Li+, Na+, K+, Cs+, as their perchlorate salt), distinctive ion-pair formation was observed depending on the nature of cations. When the fluoride complex was treated with Li+ or Na+ ion, exclusive decomplexation of the bound fluoride was observed. No appreciable interaction with K+ ion was observed. On the other hand, when the fluoride complex was treated with Cs+ ion, the cation was bound to the cup of the calix[4]pyrrole to form stable ion-pair complex. The chloride complex, on the other hand, displayed completely different complexation behavior. Namely, the Li+ ion bound to the crown moiety to form the tight ion-pair complex while the Cs+ ion bound to the cup of the calix[4]pyrrole. No appreciable interaction was observed with Na+ or K+.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-3**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Anion Binding Properties of Doubly Strapped Calix[4]pyrroles

이창희, 박자영, 엄가영

강원대 화학과

Calix[4]pyrroles have been studied as excellent anion-binding receptors since the anion-binding characteristics was discovered. Since then, various modifications have been attempted in conjunction with improving the anion binding properties. As part of the continuing efforts for enhancement of affinity and selectivity, we have now synthesized new strapped calix[4]pyrrole systems bearing two diametric straps on each side of the calix[4]pyrrole. The synthesis was accomplished by acid-catalyzed condensation of bis-dipyrromethanes and acetone. The identity of the products was fully characterized by spectroscopic means including proton NMR, HRMS and single crystal X-ray crystallography. The binding studies indicate that the titled receptor is excellent fluoride selective receptor with high affinity. The detailed studies will be presented.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-4**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Non-Aromatic, meso-Malonylidene Porphyrins: Synthesis and Chemical Properties

이창희, 이혜영, 정승두

강원대 화학과

The synthesis and characterization of non-aromatic meso-dicyanomethylidene porphyrinoid macrocycles and their expanded analogs will be described. The design and synthesis of these substances, which all contain unique exocyclic C-C double bonds at multiple meso-positions, was accomplished by utilizing a typical '3+1' type mixed-condensation. Synthesized porphyrins displayed unique protonation selectivities upon treatment with trifluoroacetic acid. The initial protonation occurred at the alpha-position on the meso substituent. The 1,4-naphthyl-thia-dicyanomethylidene porphyrin was fluorescence in spite of the non-aromatic character. The newly synthesized meso-dicyanomethylidene porphyrins displayed significantly red-shifted absorption spectra compared with those of meso-diethylmalonylidene porphyrins. The spectroscopic differences and protonation selectivity will be presented in detail.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-5**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Hybrid Calix[4]pyrroles as Molecular Recognition Motifs: Synthesis and Molecular Recognition Properties of Pyrene, TTF and Pyrrole – Containing Macrocycles

이창희, 유재덕, 박경화

강원대 화학과

We have synthesized several new modified calix[4]pyrroles bearing either fluorogenic pyrene moiety or chromogenic TTF-pyrrole moiety as a part of the mother macrocycle. The synthesized compounds were characterized by proton NMR, HRMS and single crystal X-ray crystallography. The compounds show excellent affinity toward anionic guests as well as some neutral molecules including C70 and TNT. High binding affinity was observed for fullerenes and TNT, with the detection limit of nano to micro-molar ranges. The pyrene-incorporated calix[4]pyrrole is highly fluorescence and both monoer and excimer emission are observed depending on the solvent. For example, exclusive monomeric pyrene emission is observed in toluene and excimer emission is seen in acetonitrile. The detailed binding studies with various guest molecules as well as fluorescence quenching properties will be presented.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-6**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Fluorescence Indicator Displacement 'Turn-on' Sensors for Fluoride Anion with Remarkable Sensitivity and Selectivity

이창희, Punidha Sokkalingam

강원대 화학과

Anion binding chemistry using neutral host molecules has been extensively focused due to their potential biological applications and become one of the important areas in the field of molecular recognition. We designed anionic fluorophore-bound calix[4]pyrrole that can sense fluoride anions with high sensitivity. cis-5,15-(p-fluorophenyl)-(5,10,10,15,20,20-hexamethyl)calix[4]pyrrole have been investigated as sensitive fluorometric 'TURN-ON' sensor for fluoride anion. Intense green fluorescence of coumarate anion was dissipated upon strong complexation with host. When this non-fluorescent, host-coumarate complex was exposed to the mixture of anions, the bound coumarate anion was displaced only by fluoride anion exclusively with full restoration of fluorescence. The increase in the fluorescence intensity was found to be closely related with the concentration of released coumarate anion. The remarkable selectivity and high sensitivity of the new receptor for fluoride anion is promising for real sensor applications.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-7**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Highly Sensitive, Ratiometric Fluorescence 'Turn-on' Sensor for Fluoride Anion in Organic and Aqueous Media

이창희, Punidha Sokkalingam

강원대 화학과

A simple, convenient and inexpensive method to quantitatively determine the fluoride anion concentration in acetonitrile as well as in water has been reported here. The sillyl-protected coumarin derivative was able to detect fluoride anions with high selective and sensitive turn-on chromogenic and fluorogenic dual signal by simple deprotection of sillyl moiety with tetrabutylammonium fluoride. 1H NMR titration with F- revealed the complete deprotection of sillyl group with exactly one equivalent of TBAF. UV-vis titration studies exhibited the appearance of a new intense absorption band centered at around 435 nm which was accompanied by a totally colorless to bright yellow solution, Fluorescence titration showed a new turn-on intense green emission at 500 nm, which was enhanced significantly from completely off state upon addition of F-. An easy-to-prepare test paper obtained by dipping a filter paper into an acetonitrile solution of coumarin derivative was able to detect F- in aqueous media, indicating the potential application for detecting fluoride anion in natural aqueous environments by naked eye, without the need for any spectroscopic instrumentation.

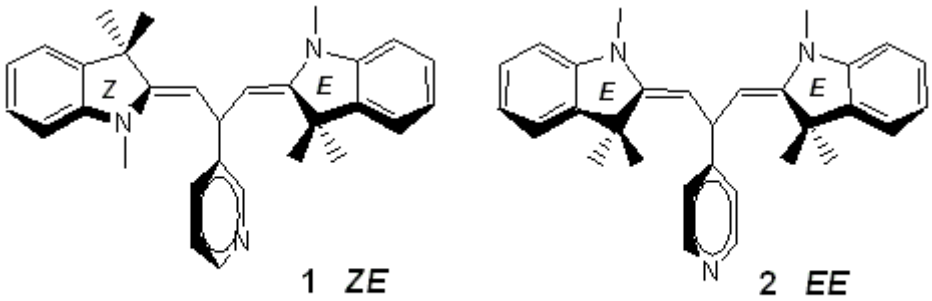
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-8**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Isomeric pyridine based leuco-TAM; synthesis and unusual stability

마소영, *금삼록

*고려대 소재화학과 *고려대 소재화학과*

Isomeric pyridine based leuco-TAM dyes, 2, 2'-(2-propane-1,3-diylidene)bis(5-chloro-1,3,3-trimethylindoline) 3- & 4-pyridinyl compounds 1-2 were prepared from the reaction of excess 5-chloro Fischer base (5-ClFB) with 3- & 4-pyridine carboxaldehyde. The X-ray crystal analysis showed that the *ZE* for 1 and the *EE* isomer for 2 are formed stereoselectively, and isomerized to *EE* or *ZE*, respectively. At equilibrium state, ^{1}H-NMR spectra of compound 1-2 showed two sets of closely-related signals, indicating the presence of the other diastereomer *ZE*/*EE*, as usual.



Major isomer

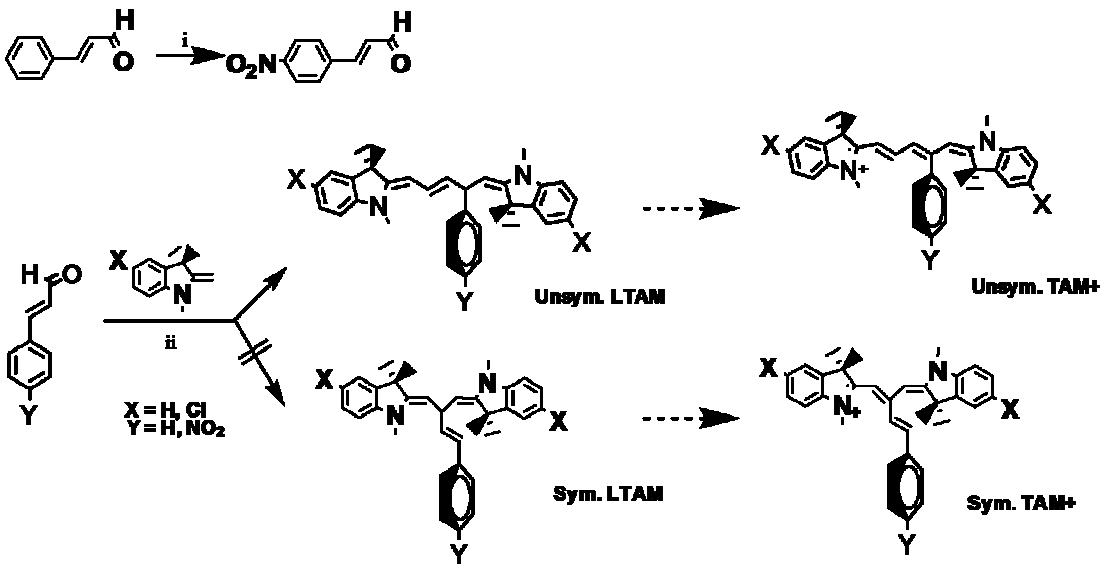
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-9**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Novel unsymmetric leuco-TAM, (2Z,2'E)-2,2'-((E)-4-(4-nitrophenyl)pent-2-ene-1,5-diylidene)bis(1,3,3-trimethylindoline) derivatives: synthesis and charaterization

김도경, 금삼록

고려대 소재화학과

Novel unsymmetric leuco-TAM, (2Z,2'E)-2,2'-((E)-4-(4-nitrophenyl)pent-2-ene-1,5-diylidene)bis(1,3,3-trimethylindoline) derivatives was prepared from the reaction of excess 5-substituted Fischer base (FB) with 4-Nitrocinnamaldehyde. None of symmetric LTAM molecules has been obtained, surprisingly. 1H NMR spectra of the synthesized unsymmetric LTAM dyes displayed very distinct signals for the five consecutive, well-separated protons in the wide range of ca 4.4-6.8 ppm, unlikely to the symmetric LTAM molecules reported earlier. The ZEE configuration of the prepared LTAM was confirmed by 2D NOESY.



i: H_2SO_4/HNO3, ii: Solvent at rt,

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-10**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of novel C-glucosides with triazine and benzotriazine ring as sodium-dependent glucose cotransporter 2 inhibitor for the treatment of type 2 diabetes mellitus

강석연, 이준원, 김민주, 김정민, 이진화

(주)녹십자 종합연구소

Novel C-glucosides bearing triazine and benzotriazine ring at distal ring position were investigated in order to develop sodium-dependent glucose cotransporter 2 (SGLT2) targeting antidiabetic agents. A variety of derivatives containing triazine and beznotriazine moieties were designed and efficiently synthesized. Several derivatives were identified as moderate inhibitors for SGLT2. The information obtained from the SAR studies in this study might help to design more active SGLT2 inhibitors that are structurally related.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-11**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

(+)-3-HM-based Polycycle Derivatives as Potential Neuroprotectants

김종엽, *김득준, 김정민, 이진화

*(주)녹십자 종합연구소 *서울대 약학대*

(+)-3-Hydroxymorphinan ((+)-3-HM) and its derivatives have shown the neuroprotective property in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) models for Parkinson's disease. During the course of its mechanism study, we found that the glutamate toxicity in HT-22 cell could be an indicator for neuroprotective property of (+)-3-HM and its derivatives. As a part of our program to identify a series of (+)-3-HM-derived comopounds that can act as a neuroprotectant, (+)-3-HM-based polycycle derivatives were prepared by intramolecular Buchwald-Hartwig cross-coupling reaction. Herein novel (+)-3-HM-based polycycle derivatives, which could be potential neuroprotective agents for neurodegenarative disease will be disclosed.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-12**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

(+)-3-HYDROXYMORPHINAN DERIVATIVES AS NEUROPROTECTANTS

공영규, 김종엽, 송광섭, 김정민, 이진화

(주)녹십자 종합연구소

(+)-3-Hydroxymorphinan ((+)-3-HM) and its derivatives have shown the neuroprotective property in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) models for Parkinson's Disease. In this animal model, daily injections with (+)-3-HM or its analogs showed that dopamine neurons in substantia nigra pars compacta have been protected and dopamine (DA) levels in striatum have been restored. As a part of exploration of a series of acyclic (+)-3-HM-based derivatives for potential neuroprotectants, we report synthesis of novel (+)-3-HM derivatives and their structure-activity relationships (SAR).

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-13**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Organosilane Multilayers Formation by Photochemical Surface Modification

Y.J. Kim, T. Ichii, K. Murase, H. Sugimura

Kyoto University

A xenon excimer lamp which irradiates vacuum ultraviolet (VUV) light at 172 nm in wavelength was applied to the photochemical surface conversion of n-octadecyltrimethoxysilane self-assembled monolayer (ODS-SAM) in the presence of atmospheric oxygen and subsequent multilayer fabrication. The terminal functional groups of ODS-SAM, $-CH_3$ groups, were converted into polar functional groups, like –COOH, by the reaction with atomic oxygen species generated photochemically through VUV excitation of atmospheric oxygen molecules. The structure of the resulting organosilane multilayer with different numbers of superimposed monolayers (from 1 to 11), prepared on a smooth and hydrophilic silicon substrate by the layer-by-layer (LbL) approach, was examined in terms of molecular organization as well as the intra- or interlayer binding modes in such novel films. Ellipsometry and grazing angle X-ray reflectivity measurements revealed that multilayer films of up to 11 discrete monolayers were successfully obtained, indicating that the self-assembly is a viable technique for the construction of relatively thick (16 nm and above) multilayer films.

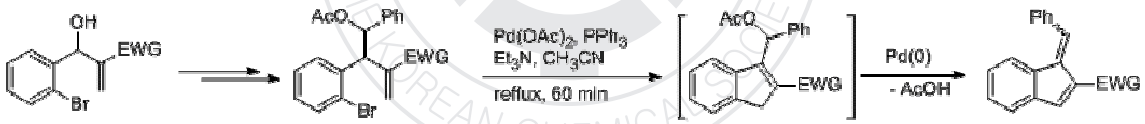
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-14**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile synthesis of benzofulvene derivatives from Baylis-Hillman adducts: In-mediated Barbier reaction combined with Pd(0)-catalyzed intramolecular Heck-elimination cascade

김고훈, 박보람, 김재녕

전남대 화학과

A facile synthesis of benzofulvene derivatives was carried out starting from the Baylis-Hillman adducts of 2-bromobenzaldehyde *via* the sequential bromination, In-mediated Barbier reaction with aldehyde, acetylation, Pd-catalyzed intramolecular Heck reaction, and the elimination of AcOH.



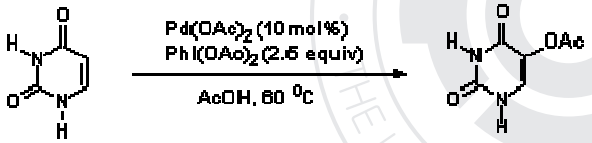
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-15**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Pd(II)-Catalyzed acetoxylation of uracil *via* electrophilic palladation

이현승, 김성환, 김재녕

전남대 화학과

A palladium-catalyzed electrophilic acetoxylation at the electron-rich 5-position of uracil was carried out. The reaction proceeded *via* the electrophilic palladation of Pd(II) at the 5-position of uracil ring, and regeneration of Pd(II) was efficiently occurred with the aid of PIDA (phenyliodonium diacetate).



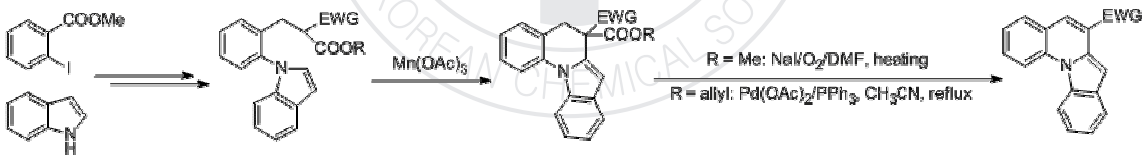
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-16**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

An expedient synthesis of indolo[1,2-*a*]quinolines *via* $Mn(OAc)_3$-mediated oxidative free radical cyclization and NaI/O_2-assisted concomitant dealkoxycarbonylation/aerobic oxidation cascade

이현승, 김세희, 김재녕

전남대 화학과

An expedient synthetic procedure of indolo[1,2-*a*]quinolines was developed using a sequential Cu-mediated *N*-arylation of indole, $Mn(OAc)_3$-mediated oxidative free radical cyclization, and NaI/O_2-assisted concomitant dealkoxycarbonylation/aerobic oxidation. The last step was replaced by a palladium-catalyzed decarboxylation/elimination protocol for the allyl ester derivatives.



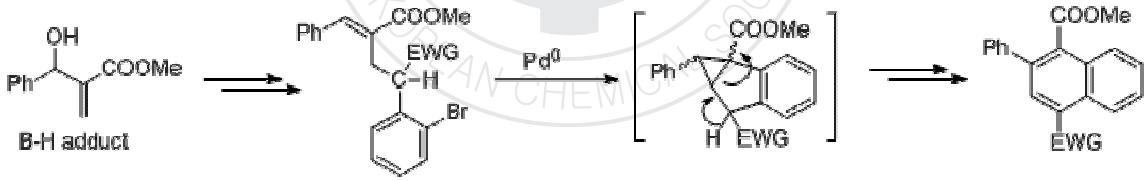
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-17**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Regioselective synthesis of naphthalenes from modified Baylis-Hillman adducts *via* a Pd-catalyzed cyclization: 5-*exo*-carbopalladation, C(sp^3)-H activation to cyclopropane, ring-opening, and aromatization cascade

김세희, 김고훈, 김재녕

전남대 화학과

Modified Baylis-Hillman adducts having 2-bromophenyl acetonitrile moiety at the primary position underwent a Pd-catalyzed cascade reaction to provide poly-substituted naphthalene derivatives in reasonable yields. The reaction involved a sequential 5-*exo*-carbopalladation, C(sp^3)-H activation to cyclopropane, ring-opening and concomitant aromatization processes.



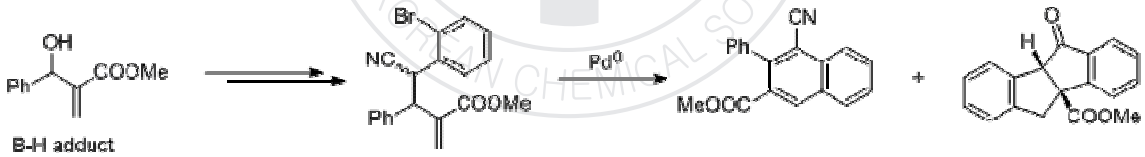
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-18**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Regioselective synthesis of naphthalenes from modified Baylis-Hillman adducts *via* a Pd-catalyzed cyclization: 6-*endo*-carbopalladation and an aerobic oxidation cascade

김세희, 이현승, 김재녕

전남대 화학과

Modified Baylis-Hillman adducts having 2-bromophenyl acetonitrile moiety at the secondary position underwent a Pd-catalyzed cascade reaction to provide poly-substituted naphthalene derivatives in reasonable yields. The reaction involved a sequential 6-*endo*-carbopalladation and a concomitant aerobic oxidation process.



일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-19**

발표분야: 유기화학

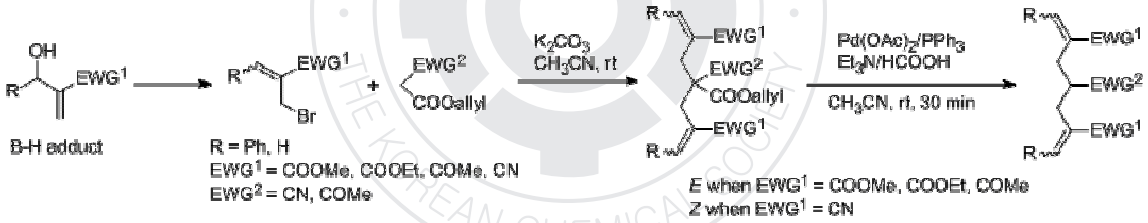
발표종류: 포스터, 발표일시: 목 10:30~12:30

An efficient synthesis of functionalized 1,6-dienes from Baylis-Hillman adducts *via* a Pd-catalyzed decarboxylative protonation protocol

박보람, 김고훈, 김재녕

전남대 화학과

An efficient synthetic procedure of functionalized 1,6-diene derivatives was developed starting from the Baylis-Hillman adducts *via* the Pd-catalyzed decarboxylative protonation as the key step.



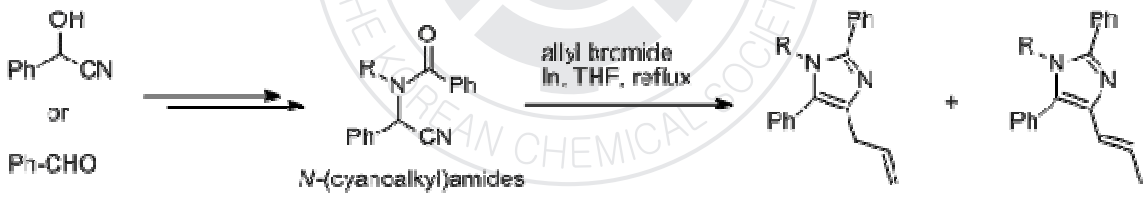
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-20**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of fully-substituted imidazoles from *N*-(cyanoalkyl)amides *via* the In-mediated allylation of nitrile and dehydrative cyclization cascade

김유미, 김성환, 김재녕

전남대 화학과

The reaction of allylindium reagents and *N*-(cyanoalkyl)amides afforded fully-substituted 4-alkenylimidazoles in moderate yields *via* the In-mediated Barbier type allylation of nitrile and the following dehydrative cyclization cascade.



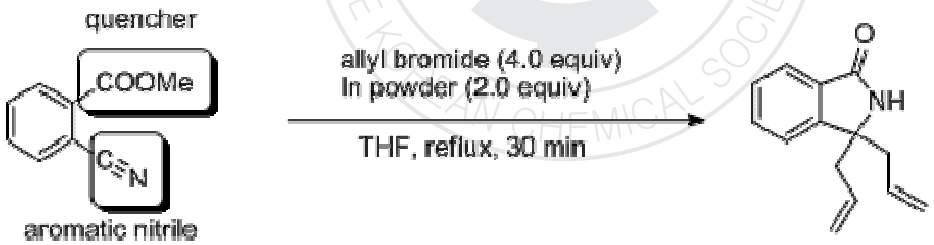
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-21**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile synthesis of 3,3-diallyl isoindolones *via* a indium-mediated double allylation of *ortho*-cyanobenzoates

김성환, 김유미, 김재녕

전남대 화학과

Various 3,3-diallyl isoindolones were synthesized *via* a indium-mediated Barbier type double allylation reaction of *ortho*-cyanobenzoates in good yields in short time. The reactivity of nitrile group toward allylindium is sufficient to form a cyclic compound when a suitable electrophilic center is present in the same molecule to trap the imine intermediate.



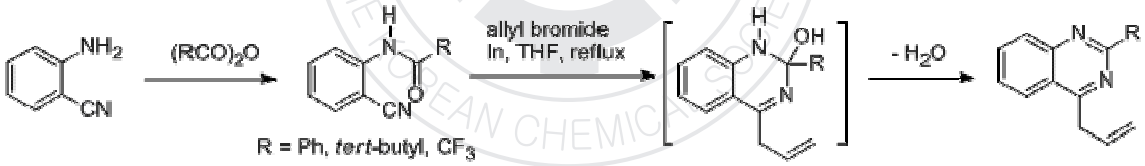
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-22**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile synthesis of 4-allylquinazoline derivatives from *N*-(2-cyanoaryl)amides *via* the In-mediated allylation of nitrile and dehydrative cyclization cascade

김성환, 김유미, 김재녕

전남대 화학과

The reaction of allylindium reagents and *N*-(2-cyanoaryl)amides afforded 2-substituted-4-allylquinazolines in good yields *via* the In-mediated Barbier type allylation of nitrile and the following dehydrative cyclization cascade.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-23**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

N-Heterocyclic Carbene-Catalyzed Intramolecular Oxidative Cyclization Reactions of 2-Alkynylbenzaldehydes

박종협, 윤소원

한양대 화학과

In the recent years, the use of organocatalyst becomes one of the promising tools for the development of new synthetic methodologies in organic synthesis. In this respect, herein we present an efficient synthesis of phthalides and isocoumarins using *N*-heterocyclic carbene (NHC) as an organocatalyst.In our study, we found that the combination of NHC and DBU effectively promoted the intramolecular oxidative cyclization reactions of 2-alkynylbenzaldehydes to give the corresponding phthalides or isocoumarins in moderate to good yields in toluene or acetonitrile as a solvent under aerobic conditions. High regioselectivities were achieved providing 5-*exo* or 6-*endo* cyclization products according to the nature of substituents at the akyne terminus.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-24**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Pd-Catalyzed *ortho*-Olefination of Acetanilides: Mechanistic Studies and Kinetic Isotope Effect

김병석, 윤소원

한양대 화학과

Recently, we have developed a Pd-catalyzed *ortho*-olefination of acetanilides under mild conditions with broad substrate scope. To gain insight into this reaction, mechanistic studies were extensively carried out. The preparation and characterization of potential intermediates such as palladacycle were achieved and the subsequent reaction with methyl acrylate underwent smoothly to give the corresponding *ortho*-olefinated acetanilide. Palladacycle could also catalyze the oxidative coupling of acetanilide with methyl acrylate to afford the corresponding ortho-olefinated acetanilide in good yield. Furthermore, kinetic isotope experiments suggest that cleavage of the C-H bond at the ortho position is involved in the rate-determining step.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-25**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

An Efficient Au(I)-Catalyzed Intramolecular Cyclization Reactions of 2-Alkenylphenyl Carbonyl Compounds

Arun R. Jagdale, 윤소원

한양대 화학과

In recent years, synthesis of indene derivatives has attracted considerable attention due to their biological activities and their presence in a variety of significant natural and synthetic compounds. Herein, we present cationic Au(I)-catalyzed intramolecular cyclization reaction to afford indene derivatives in good to excellent yields. In particular, 2-alkenylbenzaldehydes underwent intramolecular cyclization reaction to give the corresponding indenols in excellent yields, while 2-alkenylacetophenones led to the corresponding 1-methyleneindenes in good yields via dehydration.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-26**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Pd-Catalyzed Oxidative Coupling Reactions of Acetanilides with Electron-Deficient Olefins via Directed C-H Activation/C-C Bond Formation

이동진, 윤소원

한양대 화학과

Catalytic functionalization of unactivated C–H bond has become one of the most attractive research areas in modern organic chemistry. We have developed a highly *ortho*-selective Pd-catalyzed functionalization of acetanilide derivatives under mild conditions. In the present study, we have broadened the substrate scope using a variety of substituted acetanilides. The use of $K_2S_2O_8$ as an oxidant and TFA/CH_2Cl_2 as a solvent provided good yields of the products. Good yields, high regioselectivities, and broad substrate scope are the key features of this work.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-27**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Pd-Catalyzed *Ortho* Methylation Reactions of Acetanilides

장민정, 윤소원

한양대 화학과

Recently, we have developed an efficient Pd-catalyzed *ortho* methylation of acetanilides. We found that Pd(II) catalyzed effectively C-H activation and subsequent C-C bond formation regioselectively at the *ortho* position of acetanilides. Moreover, monomethylation predominated over dimethylation in this reaction protocol.

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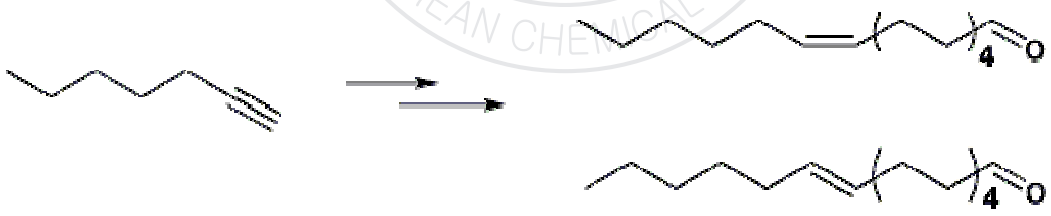
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-28**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Efficient Synthetic Method for Peach Pyralid Moth Sex Pheromone

최선희, *홍용표

*(주)그린아그로텍 부설연구소 *안동대 응용화학과*

A new synthetic method is described for the syntheses of (Z)-10-hexadecenal and (E)-10-hexadecenal, sex pheromone of Peach Pyralid Moth. Lithium acetylide of 1-heptyne was alkylated to 9-bromononan-1-ol tetrahydropyranyl ether. 10-Hexadecyn-1-ol tetrahydropyranyl ether was stereoselectively reduced over Lindlar catalyst (Ni(OAc)2/NaBH4) to give (Z)-10-hexadecen-1-ol tetrahydropyranyl ether. On the other hand, 10-hexadecyn-1-ol tetrahydropyranyl ether was reduced to (E)-10-hexadecen-1-ol tetrahydropyranyl ether by LAH. The THP ethers were deprotected and oxidized to afford the final products, (Z)-10-hexadecenal and (E)-10-hexadecenal.



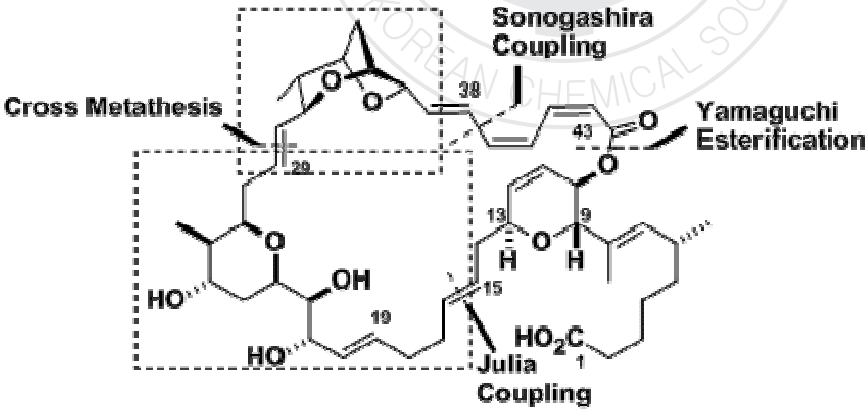
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-29**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of the C16-C29 and the C30-C37 Fragments of (+)-Sorangicin A

이성로, 이효원

충북대 화학과

Sorangicin A, a 31-membered macrolide isolated from the myxobacterium Sorangium cellulosum, shows broad antibiotic activity against Gram positive and negative bacteria. The fragment of C16-C29 was synthesized using asymmetric alkylation and allylic etherification with a rhodium catalyst. The C30-C37 fragment was prepared utilizing the Sharpless asymmetric epoxidation and the ring opening of an epoxide under acidic condition. The details of our synthetic work will be presented.



Sorangicin A

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-30**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Coupling studies of C5-C15 and C16-C26 subunits of (-)-dictyostatin

우대구, 이효원

충북대 화학과

(-)-Dictyostatin, a 22-membered antimiotic macrolide, was first isolated from the marine sponge Spongia sp. by Pettit and co-workers in 1994. It is structurally related to discodermolide. Dictyostatin inhibits the growth of human cancer cells by stabilizing tubulins. We achieved the asymmetric synthesis of C5-C15, the western part and C16-C26, the northern part of (-)-dictyostatin. Numerous methods such as the ring-closing metathesis upon silicon tethers, the Sharpless asymmetric epoxidation, the Cope elimination, and the Evans aldol reaction were utilized in the synthesis of the partial structures of dictyostatin. Synthetic details will be disclosed.

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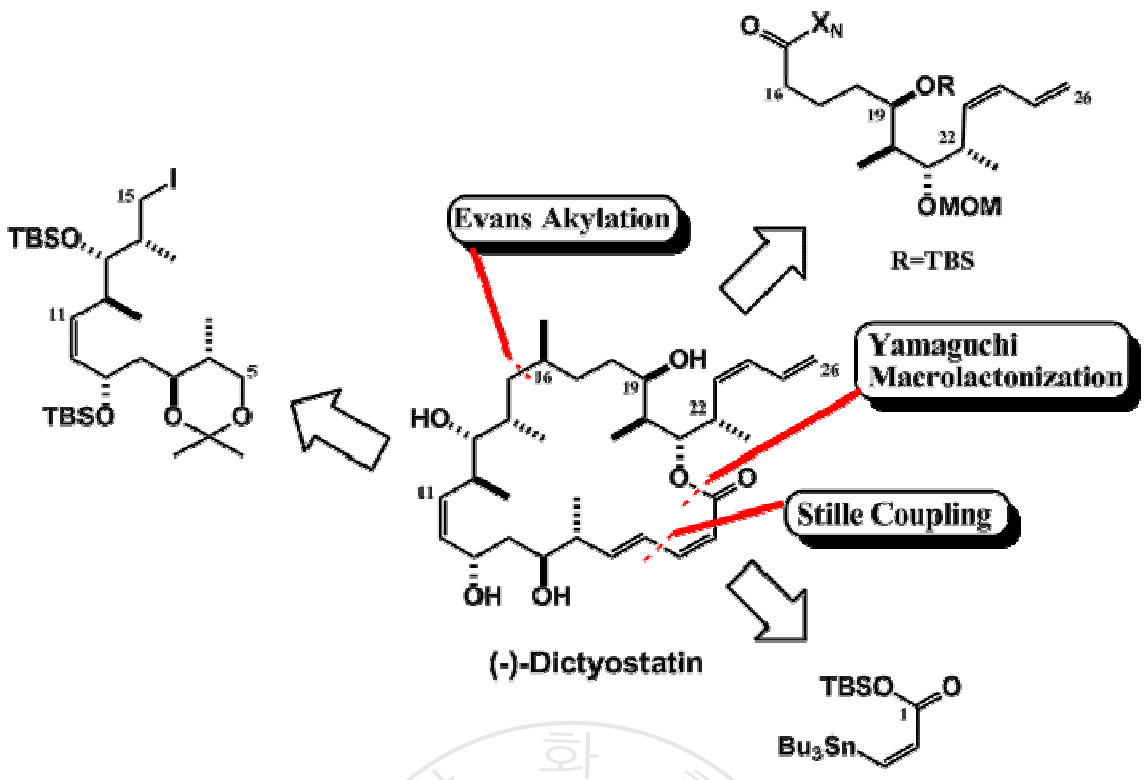


대한화학회 THE KOREAN CHEMICAL SOCIETY

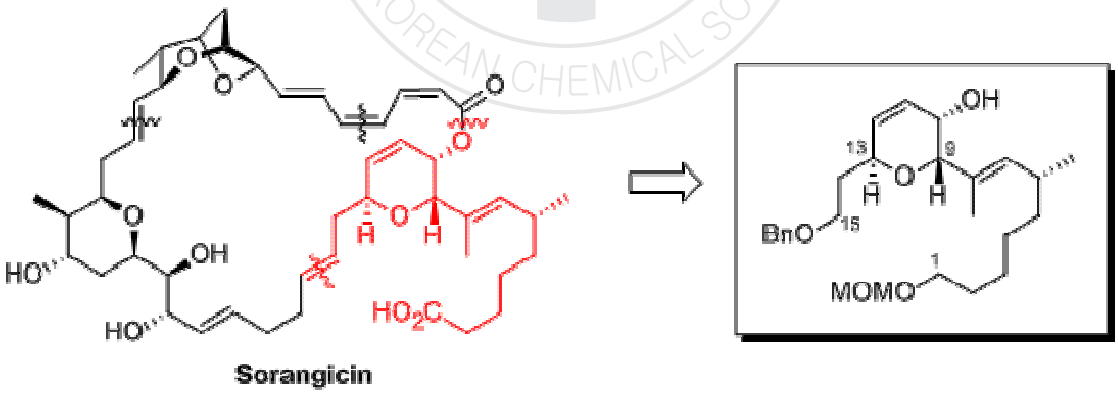
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-31**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthetic Study on the C1-C15 Fragment of Sorangicin A

양준하, 이효원

충북대 화학과

Sorangicn A is a new type of macrolide polyether antibiotic isolated from myxobacterium Sorangium cellulosum. For the C1-C15 fragment of sorangicin A, the intermediates were prepared using the RCM reaction and the Wittig reaction as key reactions. The fragment of C1-C7 of sorangicin A was prepared from 1,7-heptanediol. The subunit of C8-C15 was furnished from 1,3-propanediol as a starting material. Dihydropyranose ring was prepared using the RCM reaction from a dialkenyl ether substrate. The details of the on-going synthetic efforts will be disclosed.



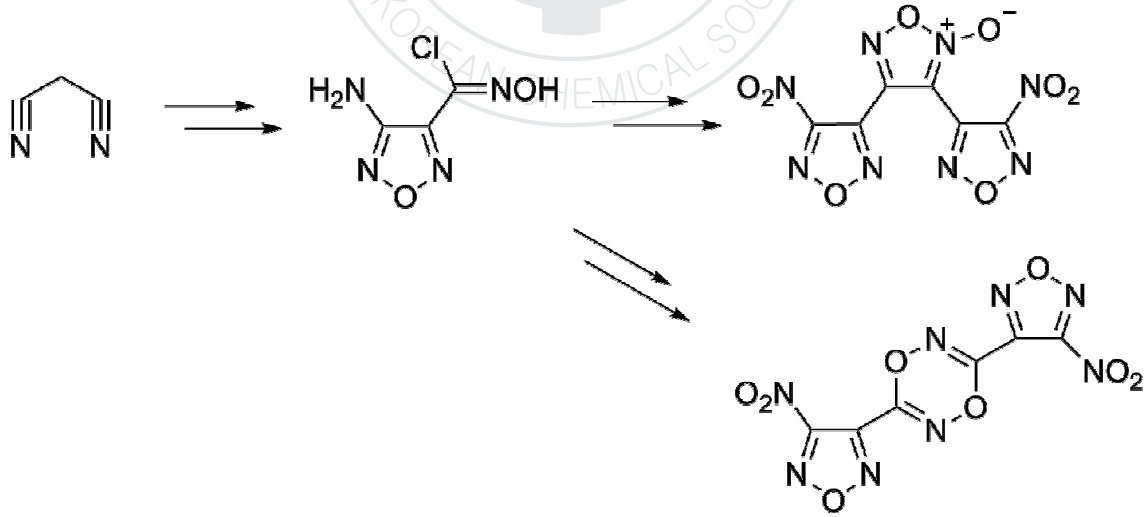
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-32**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Studies on the Synthesis and Characterization of Furoxan Derivatives

김태근, 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 (BNFF) has larger density, higher detonation velocity, and detonation pressure than HMX as a novel energetic material. The furoxan derivatives were prepared from commercially available malononitrile by multistep process, including dimerization of nitrile oxides and oxidation. We will discuss there's thermoanalytical data and some important reactions.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-33**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Asymmetric Synthesis of 3-Substituted 2-Piperazinone using Chiral Alcohol-mediated Dynamic Resolution of α-Halo Esters

장정인, 박용선

건국대 화학과

Dynamic resolution of chiral alcohol-derived α-halo esters in nucleophilic substitution reaction has been investigated. The substitution of α-halo esters with N-substituted ethylenediamine nucleophiles and following spontaneous cyclization in the presence of TBAI and DIEA provides a practical protocol for asymmetric syntheses of 3-substituted 2-piperazinones up to 95:5 er

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장소: 대구엑스코
발표코드: **ORGN.P-34**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Effective synthetic method of ketones from acid chlorides in one-pot reaction

박재교, 송주영, 안덕근

강원대 화학과

An efficient and novel methodology for various functional group transformation is important in organic synthetic fields. A ketone in the organic compound is useful undergoing a wide variety of chemical transformations, and especially development of one-pot transformation of common acid halide to ketones without isolation in mild condition is necessary in organic synthesis of various important compounds. Recently, we have found that new one-pot synthetic method of ketones from representative acid chloride in excellent yields using DIBAL and morpholine. We believe that this new method is very useful for synthesizing of ketones from acid chloride.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-35**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Efficient functional group transformations of esters to aldehydes in one-pot reaction

전아람, 길진아, 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. Aldehydes in the organic compounds is one of important functional group undergoing a wide variety of chemical transformations, and a large number of reducing agents for this purpose have been reported. Recently, we have found that a useful and new one-pot synthetic method of aldehydes from esters in quantitative yields. We believe that this new method can solve many problems for synthesizing aldehydes from esters and offer a useful methodology in organic synthesis.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-36**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Addition of Diphenyl Phosphate to Alkynes Catalyzed by Gold

박애리, 이필호, *김성각

*강원대 화학과 *KAIST 화학과*

Conversion of carbonyl compounds into enol phophates is of a great synthetic importance since enol phosphates are versatile intermediates which undergo various synthetically useful transformations. The major issue in this transformation is selectivity . Especially, the more substituted thermodynamic enol derivatives from unsymmetrical ketones normally predominate under thermodynamic conditions but to not form exclusively, which is a serious problem in organic synthesis. Thus, the preparation of thermodynamic enol phosphates as highly pure form is of synthetic importance and still a very challenging problem. We have developed the hydrophophoryloxylation reaction of alkynes using diphenyl phosphate in the presence of $Ph_3PAuCl/AgPF_6$ to afford the kinetic enol phophates. Whereas the reaction using $(C_6F_5)_3PAuCl/AgOTf$ gave the thermodynamic enol phosphates as highly pure forms. In addtion, $(C_6F_5)_3PAuOTf$ proved to be highly efficient catalyst for the isomerization of kinetic enol phosphates into thermodynamic isomers.

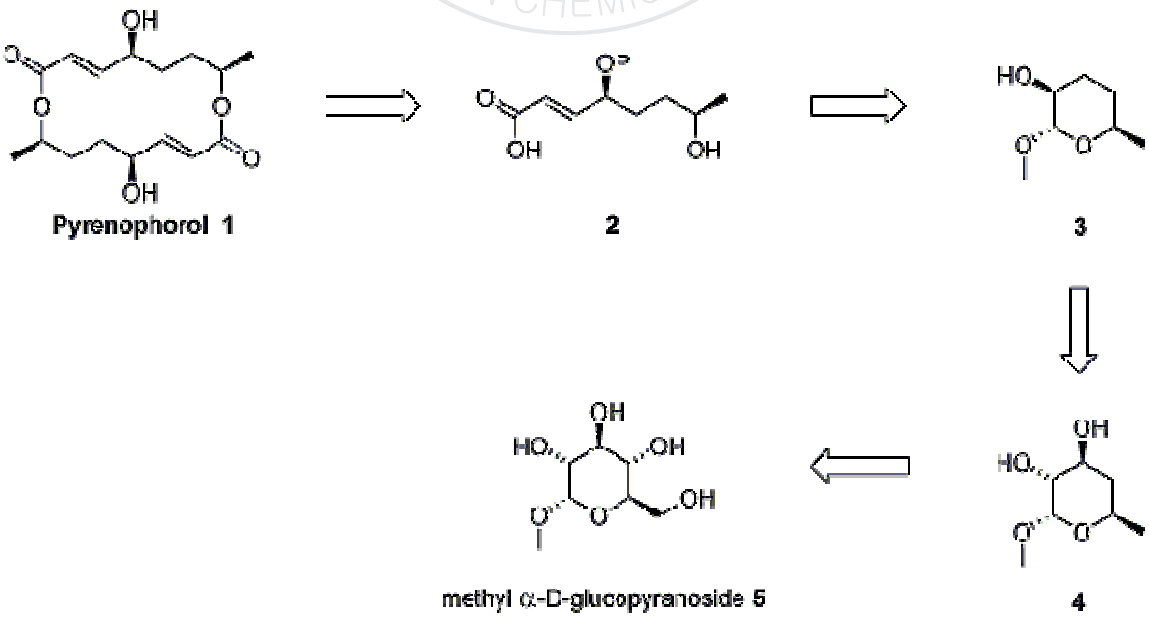
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-37**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Stereoselective Synthesis of (-)-Pyrenophorol

강한영, 오홍세

충북대 자연과학대학 화학과

Pyrenophorol (1) was isolated first from the fungus Byssochlamys niveah as well as Stemphylium radicinum. Later it was isolated from the imperfect fungus Alternaria alternate and named helmidiol which exhibits pronounced anthelmintic properties. 2We have investigated an efficient route for the synthesis of Pyrenophorol (1) starting from readily available methyl α-D-glucopyranoside. Synthesis of intermediate 4 can be easily achieved by adopting the well-reported synthetic sequence. The key compound 2 synthesized by epoxidation, epoxide opening and the Wittig reaction from the intermediate 4. Finally, the cyclization was successfully achieved using Yamaguchi esterfication to give the 16-membered lactone and protection group was removed to complete the synthesis of pyrenophorol (1).



일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-38**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of 1-Benzylpiperidin-4-one analogs and their stereochemical study using NMR spectroscopy and single-crystal XRD

Someshwar, P. Parthiban, 정연태

부경대 이미지시스템공학과

Piperidone and its derivatives are of biological interest owing to their broad-spectrum biological activities such as antibacterial, antituberculostic, antifungal, anti-inflammatory and neuronal nicotinic antagonistic activity. Their diverse biological actions are the significant factors to deal with the molecules. In this study, we have synthesized a series of compounds with 1-benzylpiperidin-4-one nucleus along with different substitutions on the piperidone heterocycle. The structural elucidation and stereochemistry of all the synthesized compounds were established by 1H and 13C NMR spectra with the use of 2D NMR correlations. Besides, the conformation of six-membered ring and orientation of the various substituents were unequivocally witnessed by single-crystal XRD analysis.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-39**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and characterization of novel Hantzsch thiazoles from 2,4-diaryl-3-azabicyclo[3.3.1]nonan-9-ones

RAMACHANDRAN, 박근수, 정연태

부경대 이미지시스템공학과

A series of 3-azabicyclic compounds ring embedded thiazoles has been synthesized by the cyclization of corresponding thiosemicarbazones with phenacyl bromide and are characterized by analytical (melting points and elemental analysis) and spectral (IR, 1H NMR, 13C NMR and Mass) techniques. Conformations of the six membered rings and orientation of the substituents have been discussed with the support of NMR data. The results show that the two bicyclic rings adopt chair conformations whereas the phenyl substituents are being oriented at equatorial positions. In addition, the reported novel Hantzsch products have been subjected to in vitro antibacterial and antifungal activity and their results are discussed.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-40**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of Aryl 3-Thiophenecarboxylates and Their NMR Studies

김수진, 이창규

강원대 화학과

Aryl 3-Thiophenecarboxylates having m- and p- substituents on the benzene ring were prepared by the reactions of 3-thienoyl chloride and m- and p- substituted phenols in methylene chloride in the presence of triethylamine. The substituent chemical shifts in chloroform-d and DMSO-d6 were examined using the Hammett correlation. The results of the correlation were compared with those obtained from similar plots with an isomeric series aryl 2-thiophenecarboxylates and those with aryl benzoates. Such comparison provided a value for aromaticity index of thiophene, which is 0.86.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-41**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis, spectral and stereochemical assignments of a series of diversely substituted 2,4-diaryl-3,5-dialkylpiperidin-4-one O-methyloximes

P. Parthiban, 정연태

부경대 이미지시스템공학과

Piperidone nucleus is present in a wide variety of naturally occurring alkaloids and exhibited a variety of biological actions. Moreover, the introduction of alkyl or aryl or halo substituents on the piperidone nucleus enhanced its activity. Similarly, the reduction of carbonyl group as oxime functionality and incorporation of substituents on it also exhibited an elevated activity. With a view of the above all, we have synthesized a series of diversely substituted 2,4-diaryl-3,5-dialkylpiperidin-4-one O-methyloximes to evaluate their antimicrobial activity. Since the stereochemistry is a major criterion for the biological actions, in this study, we established the stereochemistry of the synthesized piperidone oxime ethers with the help of COSY, NOESY and HMBC studies.

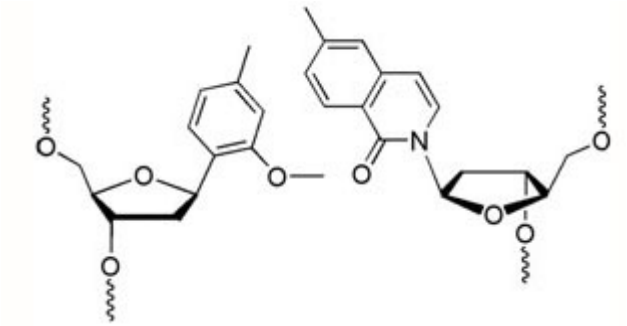
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-42**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Optimization of the hydrophobic DNA nucleobase surrogates for polymerase recognition and unnatural base pair replication

김경애, 황길태

경북대 화학과

Faithful polymerases mediated synthesis can be considered for the expansion of both the genetic alphabet and the genetic code. The stability and sequence specificity of a natural DNA duplex is based on the complementary and orthogonal Watson–Crick hydrogen-bonding patterns of dA:dT and dC:dG base pairs. Though inter-nucleobase hydrogen bonding and shape complementarity are important for the stability and faithful copying of DNA, there is no reason to assume that the pairing of two unnatural bases could not be driven by other intermolecular interactions, for example, those based on hydrophobic and van der Waals forces. Thus, much effort has been directed towards understanding the determinants of DNA stability and replication. We will present the DNA replication results of two novel unnatural base pairs in detail.



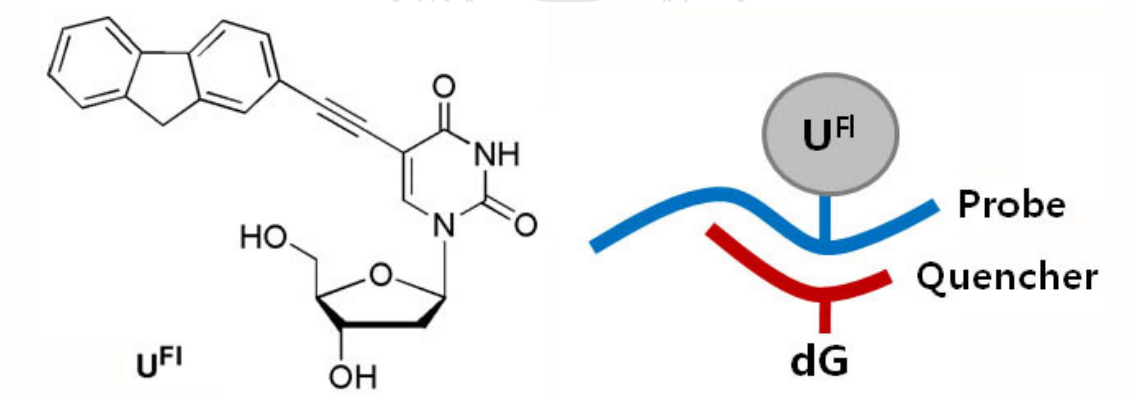
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-43**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

A Highly base-discriminating linear beacon probe containing an internal deoxyguanosine quencher

허주영, 이영애, 황길태

경북대 화학과

We have developed a new base-discriminating linear single-stranded beacon probe, minimizing the fluorescence of the probe itself by introducing dG-containing quencher that functions based on internal quenching effects. As a result of its reduced intrinsic fluorescence, this probe exhibits a drastic change in fluorescence intensity when it hybridizes with its fully matched target sequence. Furthermore, the total discrimination factors were greater than 10 for all mismatched targets in the presence of even a short (five-nucleotide) dG quencher strand, allowing the recognition of single base mismatches.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-44**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis 9,9'-diethyl-2-diphenylaminofluorene derivatives as a dopant for Blue Fluorescence in OLEDs

황진수, 이금희, *김영관, 윤승수

*성균관대 화학과 *홍익대 기초과학과*

In the past decade, organic light-emitting diodes (OLEDs) have attracted much scientific and commercial interest because of its potential application in a full-color displays in large areas. To further improvement of OLED, development of blue-light-emitting materials should be required.In this study, blue fluorescent materials based on 9,9'-diethyl-2-diphenylaminofluorene derivatives are synthesized and characterized. These materials are used as blue dopant materials for the emitting layer of organic light-emitting diode devices (OLEDs). All devices exhibit high efficiency blue emission. Especially a compound shows the maximum Luminance with 8402 cd/m^2 at 10V, Luminous efficiency 8.0 cd/A at 20 mA/cm^2 , the Power efficiency of 3.39 lm/W at 20 mA/cm^2, and CIEx,y coordinates (0.151, 0.159).

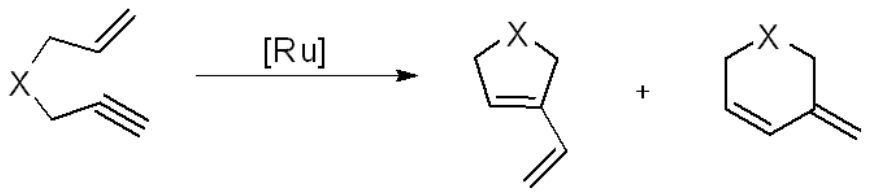
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-45**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Prevention of Undesirable Byproducts during RCEYM

송정아, 김세진, 나영임, 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

Ring-closing enyne metathesis (RCEYM) which is a variation of Ring-closing metathesis (RCM) reaction introduces a ring in compounds having an alkene and an alkyne. RCEYM yields two kinds of compounds which are exo-product and endo-product [Figure 1]. Generally, RCEYM forming 5 to 10-membered rings gives exo-products, whereas that forming 11-memebered rings or larger gives endo-products as major. In our study, RCEYM forming 5 to 10-membered rings were performed with substrates having a terminal alkene and a terminal alkyne. Exo-products and two different compounds were observed as the products. One of these two compounds was formed nearly as the same equivalent to exo-product depending on conditions. We also found that this compound was the product of the reaction between the exo-product and the catalyst. The results of our study will be discussed at the presentation in details. This work is supported by the NRF (WCU project R33-2009-000-10169-0)



X = N, O, C *exo*-product *endo*-product Figure. 1

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-46**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Marcus Theory of Leffler-Hammond Effect on Alpha for Hydride Transfer Reactions between Heteroaromatic Compounds

한인숙

강원대 과학교육학부

Rate and equilibrium constants have been determined spectrophotometrically for the reactions of a series of 1-substituted benzyl-3-carbamoyl-1,4-dihydropyridines (p-CH3, H, p-F, p-Cl, m-F, m-Cl, p-CN) with 1,3-dimethyl-2-phenylbenzimidazolium ion (BI+), 3-methyl-2-phenylbenzothiazolium ion (BT+), 5-benzylphenanthridinium ion (Ph+) and 10-methylcridinium ion (Ac+) in a solvent consisting of 4 parts of 2-propanol and one part of water by volume at 25 ± 0.1oC. The equilibrium constants, K, for these reactions range from 10-2 to 109 while the reaction constants range from 10-5 to 102. The oxidants give linear BrØnsted plots with the slopes, alphas, respectively. The alpha values vary systematically with the spontaneity of the reactions. Within the modified Marcus theory the present system presents the evidence of a parallel (Leffler-Hammond) effect on the BrØnsted Aplha. These results rationalize the one-step mechanism of hydride transfer without the intervention of high-energy intermediate.

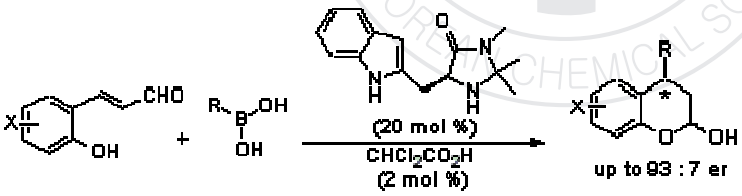
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-47**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Asymmetric organocatalytic reactions of o-hydroxycinnamaldehydes with organoboronic acids: A facile enantioselective access to chromanes and dihydrobenzopyranes

최광수, 김성곤

경기대 화학과

Catalytic asymmetric 1,4-addition reactions of organoboronic acids to o-hydroxycinnamaldehydes, which afford chromanes and dihydrobenzopyranes, have been established using an organocatalyst derived from imidazolidinone. The chromanes have been obtained in high chemical yields and enantioselectivities and can be readily used to obtain a variety of chromane derivatives through subsequent transformations.



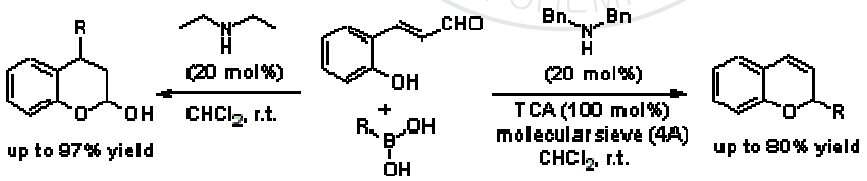
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-48**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Regioselective control of 1,2 vs 1,4 addition in organocatalytic reactions of o-hydroxy-cinnamaldehydes with organoboronic acids: A facile synthesis of 2-substituted 2H-chromenes and 4-substituted chroman-2-oles

최광수, 김성곤

경기대 화학과

The regioselective 1,2 addition and 1,4 addition reaction of o-hydroxycinnamaldehydes with organoboronic acids using an organocatalyst has been developed to afford 2-substituted 2H-chromenes and 4-substituted chroman-2-oles, respectively. Diethylamine is used as a catalyst in the 1,4 addition reaction, while dibenzylamine and trichloroacetic acid is used as a catalyst and an additive, respectively, in the 1,2 addition reaction.



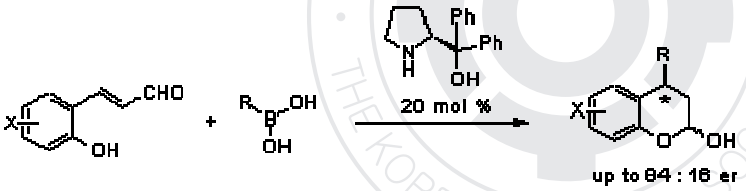
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-49**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Enantioselective Michael Addition of o-hydroxycinnamaldehydes with organoboronic acids by Organocatalyst Having Hydroxy Group

이용천, *김성곤

*경기대 자연과학부 화학과 *경기대 화학과*

Catalytic asymmetric 1,4-addition reactions of organoboronic acids to o-hydroxycinnamaldehydes, which afford 4-substituted chroman-2-oles, have been established using an organocatalyst having hydroxy group.



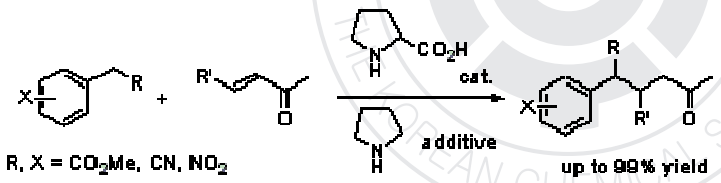
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-50**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Organocatalytic Michael addition of arylacetic ester compounds to α,β-unsaturated ketones

도정호, *김성곤

*경기대 이과대학 화학과 *경기대 화학과*

A general organocatalytic Michael addition procedure of a variety of arylacetic esters, arylacetonitriles, and arylacetocyanides to α,β-unsaturated ketones have been established. Proline and pyrrolidine is used as a catalyst and an additive, respectively, in these conjugate addition reaction.



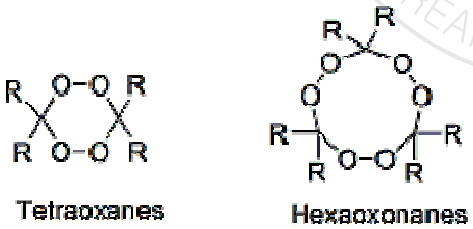
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-51**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

A New Class of α-Glucosidase Inhibitors: 1, 2, 4, 5 – Tetraoxanes and 1, 2, 4, 5, 7, 8- Hexaoxonanes derivatives

홍인석, **Ambadas B. Rode**

공주대 화학과

For the first time we assessed in vitro α-glucosidase inhibitor activity of a series of 1,2,4,5-tetraoxanes 1,2,4,5,7,8 hexaoxonanes. All tetraoxane and hexaoxonane derivatives showed 100 % inhibition at 50 µM Conc. The hexaoxonanes derivatives are more superior to the tetraoxane derivatives; moreover hexaoxonanes with longer carbon side chains show relatively good activity compared to hexaoxonanes with smaller carbon chains. The mechanistic approaches to reveal the inhibition mechanism are in progress.



R = same or different, cyclic or acyclic

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-52**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Coumarin-Based Fluorescence Turn-On Probe for Proline

김건중, 김해조

한국외국어대 자연과학대학 화학과

Higher level of proline in the blood causes a hyperprolinemia (HP-II), whose proline levels are between 10 and 15 times higher than normal, and provokes seizures or intellectual disability.[1] Thus, noninvasive analysis of the amounts of proline and its metabolites in urine is attracting a considerable interest.[2] Herein, we report a highly selective and sensitive fluorescence turn-on probe for proline. We utilized a coumarin-based aldehyhde as an aldol reactant for the selective detection of proline by a proline-catalized aldol reaction. It has been well known that proline catalyzes an aldol reaction.[3] Enamines provide a valuable alternative to the use of enolates for the selective alkylation of aldehydes.The probe has shown a selective and sensitive response to proline over other various amino acids. When proline was added, the fluorescence intensity of the probe was more than 100 times increased by proline so that micromolar concentrations of proline were detectable by the probe.Reference1. Flynn, M. P.; Martin, M. C. et al, Arch. Dis. Child. 1989, 64, 16992. Kuhara, T. J. Chromatogr. B, 2007, 855, 423. List, B.; Lerner, R. A.; Barbas, C. F. III J. Am. Chem. Soc. 2000, 122, 2395

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-53**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Hydrogen Bond-Based Fluorescent Chemodosimeter for the Selective Detection of Cyanide

박석안, *김해조

*경기대 화학과 *한국외국어대 자연과학대학 화학과*

The cyanide ion is an extremely hazardous material that damages by absorption through the lungs, gastrointestinal track, and skin and can kill mammals upon binding to a heme unit. Consequently, there is of growing interest in the development of toxic cyanide anions by fluorescent probes. Herein we report a novel fluorescent probe for the cyanide anions, which is activated by the intramolecular hydrogen bonding. The novel fluorescent probe was prepared for the selective detection of cyanide anions. Intramolecular hydrogen bond plays a critical role in the chemosensor and it is presumed to activate the carbonyl group of the conjugated enone system. The Michael addition of cyanide anion to the Michael acceptor possibly disrupts the electronic state of the probe and therefore makes the fluorescence of the probe significantly interrupted. The chemodosimeter has shown a selective and sensitive response to cyanide over other various anions through the Michael reaction. When cyanides were added, the fluorescence intensities of 1 were increased more than 100-fold so that millimolar concentrations of cyanide anions were detectable by the naked eye.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of morpholine-2-one and 1,4-oxazepan-2-one derivatives

강선영, *전근호

*숭실대 화학과 *숭실대 화학*

Morpholine-2-one and 1,4-oxazepan-2-one derivatives were applicated in important clinical trials and fuel industry. However, their synthesis was known to be complicated in moderate yield. We tried to synthesize morpholine-2-one and 1,4-oxazepan-2-one via regioselective chloroacetylation of 2-aminobutane-1,4-diol derivatives. We found regioslectivities in chloroacetylation of *N*-protected 2-aminobutane-1,4-diol were depend on the nature of *N*-protecting groups, acylating reagents, and metal chelating reagents. When sulfonates for *N*-protecting group and chloroacetyl anhydride were used, 3-amino-4-hydroxybutyl 2-chloroacetate was prepared regioselectivity. On the other hand, when *t*-butoxycarbonyl(Boc) for *N*-protecting group and chloroacetyl anhydride were used, 2-amino-4-hydroxybutyl 2-chloroacetate was obtained in high yield. When *N*-Boc-2-amino-1,4-diol was reacted with chloroacetyl chloride in preserve of $ZnCl_2$ and pyridine, *N*-Boc-2-amino-4-hydroxybutyl 2-chloroacetate was produced as a only product. Intramolecular cyclization of 2-amino-4-hydroxybutyl 2-chloroacetate and 3-amino-4-hydroxybutyl 2-chloroacetate effectively gave morpholine-2-one and 1,4-oxazepan-2-one derivatives in mild conditions.

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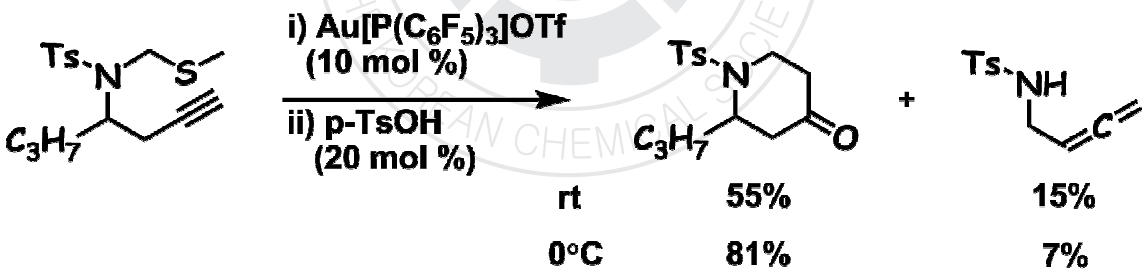
발표종류: 포스터, 발표일시: 목 10:30~12:30

Gold(I)-catalyzed of Homopropargylic Thioalkoxy Amine

김철재, 이영호

포항공과대 화학과

We developed a formal alkyne aza-Prins reaction via gold(I)-catalyzed cyloisomerization of mixed N,O-acetals. Now, we try to expand the scope of this with mixed N,S-acetals, based on the difference of nucleophilicities of O and S. In case of mixed N,S-acetals, aza-Cope rearrangement has seriously arisen for the activation of thioether, unlike the case of mixed N,O-acetals. And, here includes a formal synthesis of racemic coniine.



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Novel Electrochemiluminescent Dinuclear Ru(II) Complexes Bridged With Ether-linked Dibipyridyl Ligand

한해리, 오현주, *강창훈, *이원용, 김병효

*광운대 화학과 *연세대 화학과*

Electrochemiluminescence (ECL) is a well-known method for generating light. Organometallic eletrophosphoresent materials become important for ECL. Since the discovery of the ECL of $[Ru(bpy)_3]^{2+}$ (bpy=2,2'-bipyridine), this metal complex have been used as a sensitive and selective detection method for the analysis of a wide range of compounds.In our previous studies, we have synthesized ruthenium(II) complexes containing various α-diimine ligands for developing more sensitive and efficient electrochemiluminescent ruthenium(II) complexes. Since the solubility of these ruthenium complexes is important for improving ECL efficiency, we designed new dinuclear ruthenium complexes that were linked with ether-linked bridging ligands. Thus, new ether-linked bridging ligands (bpy-(CH_2-O-CH_2-O-CH_2)-bpy) were prepared. Then, a series of novel ruthenium(II) complexes such as $[Ru(L)_2(BL)Ru(L)_2](PF_6)_4$ (BL : bpy-(CH_2-O-CH_2-O-CH_2)-bpy ; L : bpy, o-phen, DTDP) were synthesized and characterized on the basis of ^{1}H NMR and MALDI-TOF mass data. Their electrochemical redox potential, UV, PL, and ECL were investigated for the application as well. As a result, dinuclear ruthenium(II) complexes containing ether-linked bridging ligands were observed as high as 1.6 fold greater than that of $[Ru(o\text{-}phen)_3](PF_6)_2$.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Reductive heterocyclization to benzimidazoles using indium/AcOH

김지혜, 김재호, 전영무, 김병효

광운대 화학과

Benzimidazoles have been widely investigated as useful compounds in pharmaceuticals, such as anti-HIV, anti-microbial and anti-inflammatory. We have developed the various reductive heterocyclizations using indium-metal because of its green chemistry characteristics and those are also applicable for the benzimidazole synthesis. Thus, based on our previous success, we examined one-pot benzimidazole synthesis via indium-mediated reductive heterocyclizations of 2-nitroanilines with trimethyl orthoalkylates. As we expected, heterocyclization reactions of 2-nitroanilines with trimethyl orthobenzoate or trimethyl orthoacetate using indium/AcOH in ethyl acetate at reflux produced excellent yields of the desired benzimidazoles. Herein, we report the reductive heterocyclization to benzimidazoles using indium/AcOH.

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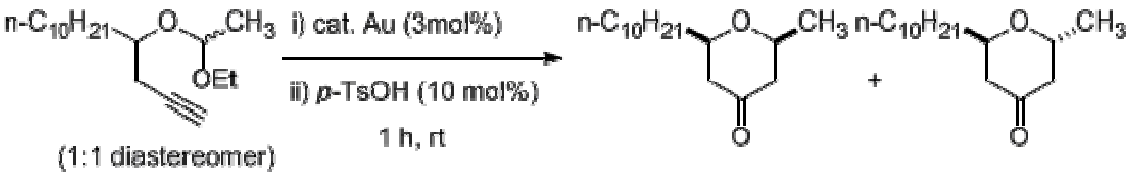
Gold(I)-Catalyzed Cycloisomerization of O,O-Acetals Generated from Homopropargylic Alcohols to Highly Substituted Tetrahydropyran-4-ones

배효진, 이영호

포항공과대 화학과

Recently, we have developed a new method for the synthesis of highly substitutued cis-2,6-tetrahydropyranones through gold(I)-catalyzed cycloisomerization of 4-(alkoxyalkyl)oxy-1-ynes as key event, which features catalytic model of Petasis-Ferrier rearrangement.1 In this cycloisomerization, it is noteworthy that diastereoselectivity of highly substitutued 2,6-tetrahydropyranones is significantly affected by ligand effect of cationic (tri-alkylphosphine) gold complexes. The synthetic utility of this method is expanded by dihydroxylation of cycloisomerized intermediate, enol ether, to 3-hydroxy-2,6-tetrahydropyran-4-one as a single diastereomer.



cat.	yield		
$Au[P(C_6F_5)_3]^+SbF_6^-$	57%	:	28%
$Au[P(C_6H_5)_3]^+SbF_6^-$	63%		13%
$Au[P(t\text{-}Bu)_2(o\text{-}Ph)Ph](CH_3CN)^+SbF_6^-$	72%	:	9%

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Arylamine Substituted DPVBi Derivatives for Efficient Blue Light-Emitting Materials

오수현, 이금희, *김영관, 윤승수

*성균관대 화학과 *홍익대 기초과학과*

Organic light-emitting diodes (OLEDs) have been developed for full color displays. However, they still need more efficient blue light-emitting materials due to their potential application. DPVBi is known to be a highly efficient blue-emitting material for electroluminescent devices. In this study, we have designed DPVBi derivatives introduced arylamino groups to improve the efficiency of devices. A series of arylamine substituted DPVBi derivatives with various aromatic systems were synthesized via the Horner-Wadsworth-Emmons. Among those, a derivative exhibits a high-efficiency blue emission with the maximum luminance of 7,005 cd/m^2 at 10 V, the luminous efficiency of 6.24 cd/A, and power efficiency of 2.63 lm/W at 20 mA/cm^2. The peak wavelength of the electroluminescence was 454nm with the CIE x,y coordinates of (x = 0.151, y = 0.143). Especially, the derivative with N- diphenylamine group performs high electroluminance. It shows the maximum luminance of 16,110 cd/m^2 at 10 V, the luminous efficiency of 10.1 cd/A at 20 mA/cm^2, power efficiency of 4.08 lm/W at 20 mA/cm^2, and the CIE x,y coordinates of (x = 0.197, y = 0.358) at 10 V.

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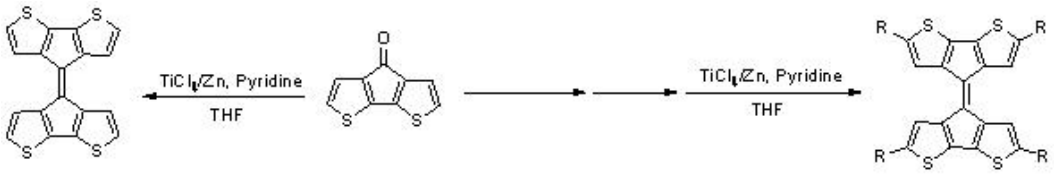
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Properties of New fused heteroacene for OTFTs

정희정, 박지희, 천은정, 안진영, 김현진, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Organic field - effect transistors (OFETs) based on organic semiconductors have attracted great attention because of their potential applications in low - cost, lightweight, and flexible large - area plastic circuits, such as flat display, electronic papers, and smart memory/sensor elements.Fused acenes are good for semiconductor because of their excellent electronic properties, stability under ambient conditions, and ease of chemical modification. And also fused acenes have high charge - carrier mobility and excellent optical properties.Therefore we designed dimerized fused heteroacene small molecules for electronic materials and synthesized with simple methodology. The synthesized molecules have more conjugated double bonds not by length, but the width. Herein we report synthesis and characterization of new dimerized heteroacene for OTFTs.



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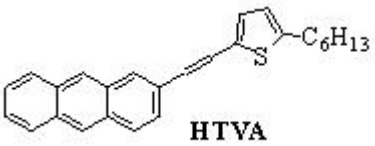
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Characterization of Thiophene-containing Anthracene Derivatives

박지희, 정희정, 천은정, 안진영, 김현진, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Organic field-effect transistors (OTFTs) have recently received great attention due to the potential for low-cost, large-area, flexible, and lightweight electronic devices, such as active-matrix flat display, electronic paper, radio frequency identification tags, and sensors.In the studies, thiophene-based materials are proposed to have good OTFT performance due to various intra- and intermolecular interaction, including weak hydrogen bonding, π-π staking and sulfur-sulfur interaction. And extended acene such as anthracene and pentacene enhance the intermolecular overlap of organic semiconductors in the solid state and lead to high field-effect mobility.We wanted to improve the charge carrier mobility. So, we designed and synthesized a series of anthracene derivatives. We will reported the characterization for new anthracene derivatives.



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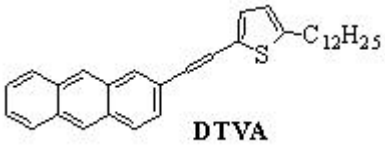

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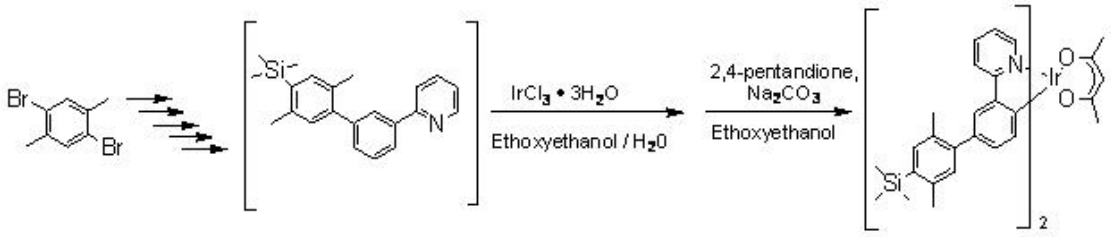
Synthesis of New Iridium Complex for OLEDs

안진영, 박지희, 정희정, 천은정, 김현진, 김윤희, 이상경

경상대 화학과

Among of the reported phosphorescent heavy-metal compounds cyclometalated iridium (III)complexes have emerged as the most promising materials for high performance work.The device efficiency and emission color of iridium-based OLEDs can be modified easily by tuning the structure of the organic-ligand chromophore. A variety of iridium complexes have been synthesized, basically containing two cyclometalated ligand and a single monoatomic bidentate ancillary ligand or with three cyclometalated ligand. So, we decided to prepare new iridium complex by reaction Ir(acac) with 2-(biphenyl-3-yl)pyridine and trimethylsilyl functional group. In practically, triarylsilyl moieties are known for high stability as well as solubility, and thus give improved efficiency. And cyclic ligands are good stability, a rapid response time and access to colors across the visible spectrum.In this poster, we want to report the electrochemical, electroluminescence properties of new synthesized iridium complex.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

A Novel p-Type conjugated polymer: Synthesis, and Characterization

강문성, 이민정, 강소희, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Polymers and conjugated oligomers 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. Among them, thiophene-based polymers have shown highest mobility with high crystalline orders on the substrate. For example, regioregular head-to-tail poly(3-hexylthiophene)s (P3HT) with mobility of 0.1 cm2/Vs. However, development of new polymeric semiconductors with better performance is still required. In this research, we designed new semiconductors material.The obtained polymer was characterized by various spectroscopic methods such as IR and NMR. The thermal, optical and electrical properties of polymer were also investigated.

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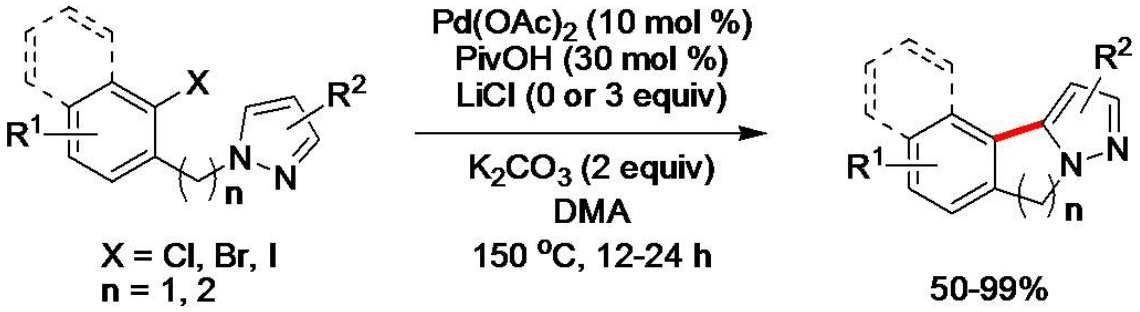
발표종류: 포스터, 발표일시: 목 10:30~12:30

Palladium-Catalyzed Intramolecular C-H Bond Activation of Pyrazoles

최영록, *허정녕

*고려대 화학과 *한국화학연구원 신약연구단*

One of the most attractive methods for forming C-C bonds with a catalytic system is through C-H bond functionalization. Transition-metal catalyzed transformations represent a central strategy in this respect, and in particular Pd catalyzed reactions play a pivotal role. In connection with our ongoing studies in the synthesis of biologically important heterocyclic compounds, which possess a pyrazole motif, we became interested in exploring the intramolecular C-H bond activation of pyrazole scaffolds. Although elegant approaches of C-H bond activation of pyrazoles have been developed, intramolecular C-H bond activation of pyrazole motifs is somewhat limited. Herein, we have established a novel, direct, onestep synthesis of pyrazolo[5,1-*a*]isoindoles via Pd-catalyzed intramolecular C-H bond activation. The use of LiCl was found to be essential in these reactions, to suppress further C-H bond activation at the C3 position of pyrazolo[5,1-*a*]isoindole when the pyrazole is unsubstituted. Furthermore, we have applied this protocol to the synthesis of pyrazolo pyrazolo[5,1-*a*]isoquinolines possessing a six-membered central ring system. Fully substituted pyrazolopyrazolo[5,1-*a*]isoindole was also synthesized by using sequential intra- and intermolecular C-H bond activation.



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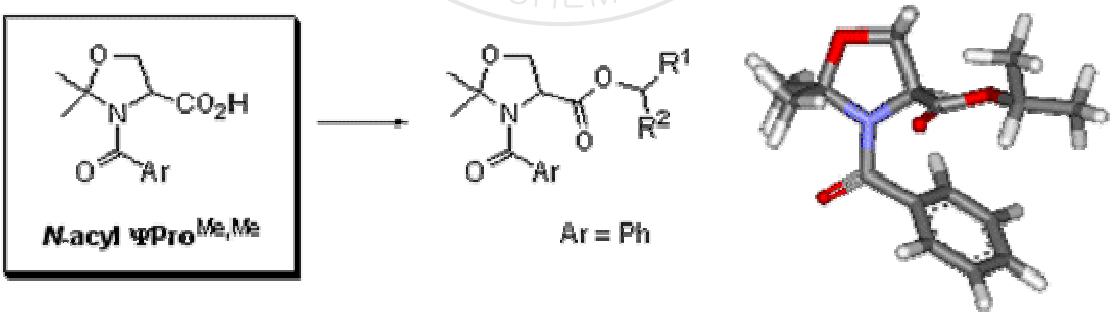
N-Acyl Pseudo-prolines as Chiral Derivatizing Agents for the Determination of the Absolute Configuration of Secondary Alcohols

한소영, 최기항

고려대 화학과

New chiral auxiliary reagents, 3-acyl-2,2-dimethyloxazolidine-4-carboxylic acids (N-acyl pseudo-prolines), have been prepared from serine and acyl chlorides through a simple short-step synthesis. The pseudo-proline esters of chiral secondary alcohols showed significantly different 1H NMR chemical shift values depending on the stereochemistry of the derivatizing agent. This chemical shift difference could be correlated to the absolute configuration of the substrate alcohol following proper conformation analysis. Preparation of more efficient reagents with larger chemical shift differences could be achieved simply by using acyl groups with stronger anisotropic effects.



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Alkyl quinoline-3-carboxylates from Baylis–Hillman acetates of 2-azidobenzaldehydes

김혜정, 이기정

한양대 화학공학과

A simple method for the synthesis of several alkyl quinoline-3-carboxylates using iminophosphorane-mediated cyclization reactions of 3-(2-azidophenyl)-2-nitromethylpropenoates has been described. These compounds were readily obtained from the Baylis–Hillman acetates of 2-azidobenzaldehydes using sodium nitrite.

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2-Alkoxy-3-cyanomethylquinolines from Baylis–Hillman acetates of 2-azidobenzaldehydes

정은미, 이기정

한양대 화학공학과

A simple method for the synthesis of several 2-alkoxy-3-cyanomethylquinolines using iminophosphorane-mediated cyclization reactions of 3-(2-azidophenyl)-2-cyanomethylpropenoates has been described. These compounds were readily obtained from the Baylis–Hillman acetates of 2-azidobenzaldehydes using potassium cyanide.

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Synthesis of Chalcone Derivatives and Comparison of their Antioxidant Effects

김미란, 전종갑

한림대 화학과

Chalcones are important bioactive compounds. They show antibacterial, antifungal, antitumor, anti-inflammatory and anti-oxidant effect properties. It has been known that the chalcone compound has superior anti-oxidant effects due to their A ring's catechol structure and B ring's resocinol structure. To confirm these unique structural properties, we changed the hydroxyl positions in chalcones preparing by aldol-condensation using acid or base conditions. The prepared compounds are compared in their anti-oxidant effect using DPPH, ABTS and Tyrosinase inhibitory methods.

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Synthesis of Benzophenone-Benzoate Derivatives and their Anti-Inflammatory Effects

권은미, 전종갑

한림대 화학과

Benzophenone-benzoate 구조의 화합물들은 prostaglandin H synthase 에 의해 나타나는 arachidonic acid 로 인해 항염증 작용을 나타낸다고 알려져 있다. Prostaglandin 은 염증을 자극하고 지방조직에서 지방분해를 방지한다고 알려져 있다. 다양한 구조의 benzophenone-benzoate 화합물들을 DCC coupling 과 $AlCl_3$ 를 이용한 Fries rearrangement, S_N2 등의 방법을 이용하여 총 3 step 의 합성 방법을 개발하였고, 합성한 화합물들을 MTT assay 와 nitrogen oxide 의 발생억제를 통한 항염증 효과를 측정하였다.

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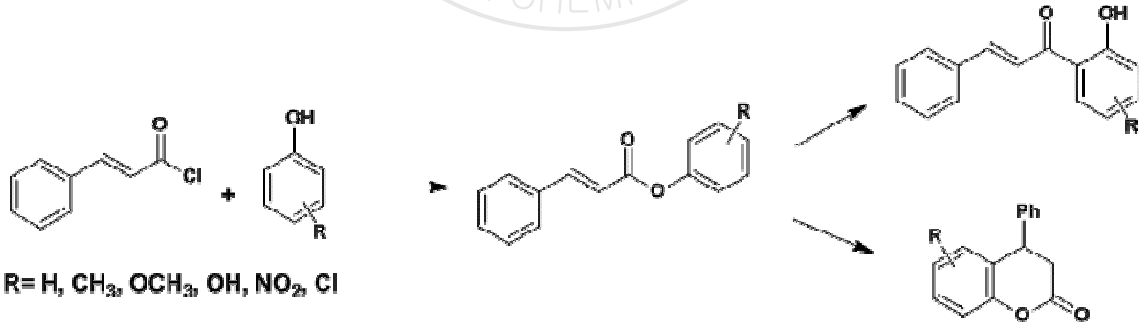
장소: 대구엑스코
발표코드: **ORGN.P-70**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Selective Syntheis of Dihydrocoumarins or Chalcones from Aryl Cinnamates

양덕모, 전종갑

한림대 화학과

Chalcones show varieties of antibacterial, antifungal, antitumor and anti-inflammatory properties. Some chalcones demonstrated the ability to block voltage-dependent potassium channels. They are intermediates in the biosynthesis of flavonoids, which are substances widespread in plants. Many synthetic methods for 4-aryl-3,4-dihydrocoumarins have been reported up to the present, but most of the procedures based on the condensation of phenols with cinnamic acids in strong acidic media and at high temperature. In this study, dihydrocoumarin and chalcone derivatives are prepared selectively from aryl cinnamates by using intramolecular cyclization or Fries rearrangement, respectively.



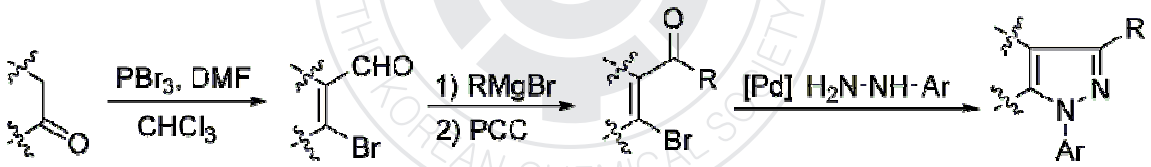
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-71**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Palladium-Catalyzed Synthesis of 3-Alkyl-1-aryl-1H-pyrazoles from β-Bromovinyl Ketones and Arylhydrazines

이혜경, 조찬식

경북대 응용화학과

β-Bromovinyl ketone are cyclized with an array of arylhydrazines in toluene in the presence of a palladium catalyst and a phosphorous chelating ligand along with NaOtBu to give 3-alkyl-1-aryl-1H-pyrazoles in moderate to good yields.



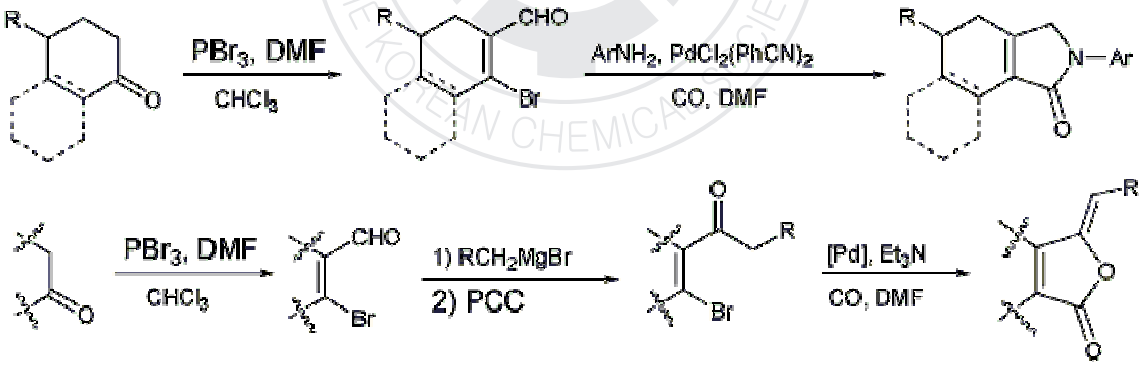
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-72**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Palladium-Catalyzed Synthesis of Hydroisoindol-1-ones and (Z)-Alkylidenefuranones from β-Bromvinyl Aldehydes and Ketones

김효보, 조찬식

경북대 응용화학과

β-Bromovinyl aldehydes react with anilines under carbon monoxide pressure in DMF in the presence of a catalytic amount of a palladium catalyst to give the corresponding hydroioindol-1-ones in good yields. ′ -Bromovinyl ketones are cyclized to (Z)-alkylidenefuranones in good yields under carbon monoxide pressure in DMF in the presence of a catalytic amount of a palladium catalyst.



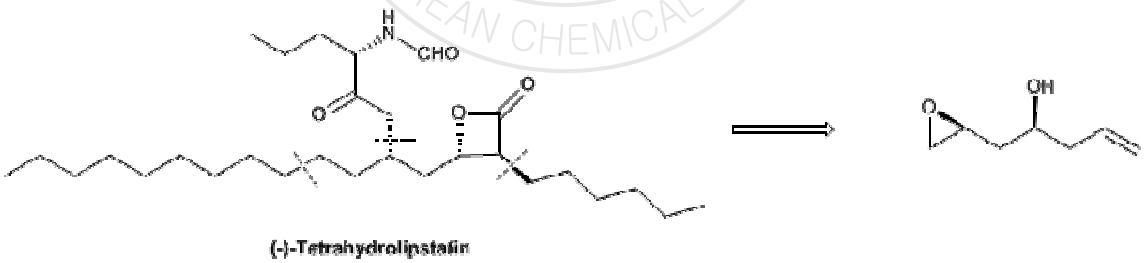
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-73**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthetic Studies of (-)-Tetrahydrolipstatin

최경환, 김혜미, 태진성

연세대 화학과

(-)-Tetrahydrolipstatin(THL) is an anti-obesity drug marketed under tradename of Xenical or Orlistat internationally. THL is a saturated derivative of natural product lipstatin isolated from *Streptomyces toxytricini* in 1987 and has a β-lactone moiety that can react with pancreatic lipase enzyme. We have tried to synthesize (-)-THL from an enantioenriched (*S,S*)-epoxy alcohol generated by hydrolytic kinetic resolutions(HKR) method using Jacobson's catalyst. From the (*S,S*)-epoxy alcohol, β-lactone structure was established via epoxide ring opening and lactonization strategy. We expected that saturated-carbon chain of (-)-tetrahydrolipstatin could be achieved by enantioselective α-alkylation and cross metathesis.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-74**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

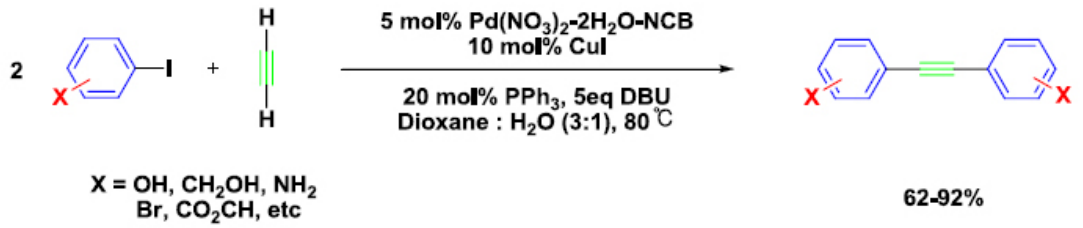
Synthesis of Functionalized Bisarylacetylene Derivatives from Acetylene Gas OverNano-sized Carbon Ball Supported Palladium Catalyst

손종우, *김경만, **이철위, 염을균

*충남대 화학과 *한국화학연구원 에너지소재센터 **한국화학연구원 신화학연구단*

Functionalized diarylacetylenic compounds are valuable intermediates in organic synthesis of natural products, pharmaceuticals, synthetic agrochemicals, and molecular materials. Although Sonogashira cross-coupling with substituted terminal acetylenes has been shown to be a powerful synthetic method for disarylacetylenic compounds, only a few literature sources have reported diarylation coupling reactions with acetylene gas. Recently, many research groups are interested in developing environmental friendly non-halogen anti-flammable materials due to environmental issues. In this research, we studied efficient synthetic method for the diarylacetylene compounds, and the synthetic method can be applied for the preparation of polyaromatic compound for material science. We obtained symmetrical diarylacetylene compounds by using palladium nitrate on nano carbon ball(NCB), which catalyst is able to recyclize in 5 times without any significant loss.

Synthesis of Functionalized Bisarylacetylene Derivatives from Acetylene Gas over Nano-sized Carbon Ball Supported Palladium catalyst



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-75**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Copper free-Sonogashira cross-coupling reaction with heterogeneous palladium catalyst

손종우, *김경만, **이철위, 염을균

*충남대 화학과 *한국화학연구원 에너지소재센터 **한국화학연구원 신화학연구단*

Sonogashira cross-coupling reaction is efficient route to make a bond between sp-carbon and sp2 carbon, basically using palladium catalysts, copper catalyst, ligand, and inorganic or organic bases. This reaction has been developed in many ways, palladium-free, copper-free, ligand-free, solvent-free(ionic liquids) conditions. However, many reports containing Sonogashira cross-coupling reaction with terminal alkyne(phenyl acetylene) have reported that homocoupling process is unavoidable due to copper catalyst. So, we report that Sonogashira cross-coupling reaction, with recyclable palladium catalyst supported on nano-sized carbon ball(also copper-free condition), is able to efficiently synthesize a desired product.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-76**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

New Synthetic Method of Functionalized Organotrifluoroborates via 1, 3-Dipolar Cycloaddition Reaction

Bolla Krishnavenu, *김동수, **박순혜, ***함정엽

*과학기술연합대학원대 Dept.of Med.Chem. *강릉대 화학과 **KIST 천연물소재센터 ***KIST 천연물소재연구센터*

Recently, potassium organotrifluoroborate salts have been used as important synthetic reagents in the Suzuki-Miyaura cross-coupling reaction. Potassium organotriflouroborates are easily prepared by the addition of inexpensive KHF2 to various organoboron intermediates, and they are stable to air and moisture. As part of a study to prepare functionalized potassium organotrifluoroborates, we were pleased to discover that 1,2,3-triazole-containing organoaryltriflouroborates are readily obtained via one-pot 1, 3-dipolar cycloaddition reaction (click chemistry) with haloaryltrifluoroborate and alkyne. In this presentation, detailed mechanistic considerations will be described.

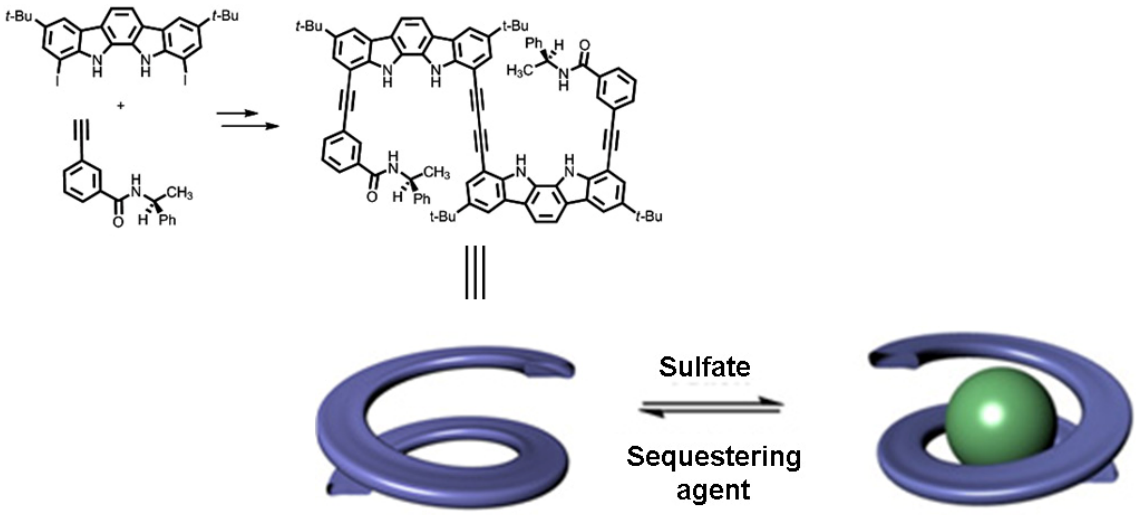
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-77**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Reversible Helical Inversion of Indolocarbazole-Based Chiral foldamer by

석재민, *Liu Xinfang, **나명수, 정규성

*연세대 화학과 *한양대 응용화학과 **울산과학기술대 친환경에너지공학부*

Introduction of chiral moiety in helical foldamer scaffold is in existence as biased helical structure by energy difference between *M*(left)- and *P*(right)-helix. Accordingly, helical chiral foldamer is possible to apply as molecular switch if it is able to control the helicity.Herein, we synthesized indolocarbazole based foldamer which was controlled helicity by chiral termini. Through intramolecular hydrogen bonding between indolocarbazole NHs and carbonyl groups of chiral moiety, foldamer preorganized biased helical conformation. By in addition of sulfate ion, helicity was inverted. Further, we controlled chiral helicity using sequestering agent such as stronger sulfate binding foldamer reversibly. Helicity control of chiral foldamer was proven by 1D-, 2D-NMR, CD and X-ray single crystallography studies.



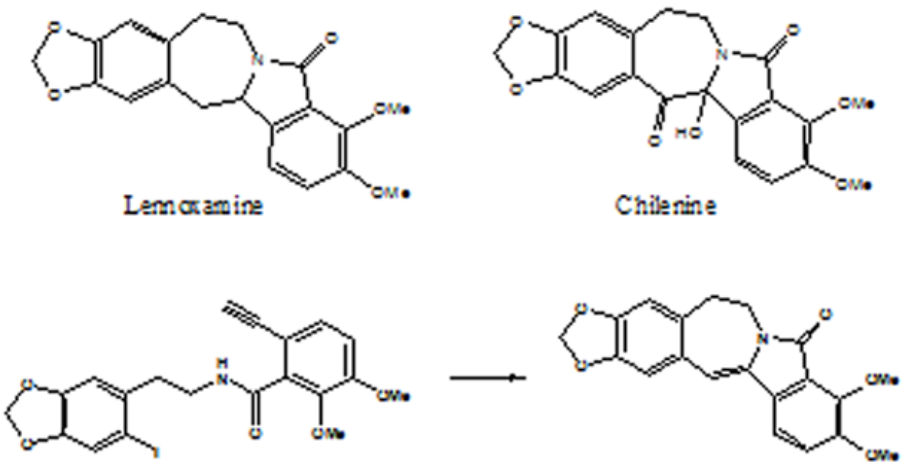
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-78**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Study on the heterocycle formation using a palladium catalyst : Application to the syntheses of lennoxamine and chilenine

오금록, 김건철

충남대 화학과

Isoindolobezazepine alkaloids, lennoxamine and chilenine, isolated from the plants of the Chilean Berberis species, are a new class of alkaloids belonging to the aporhoedane series. Although these alkaloids do not have important biological activities, their unique structure feature, five- and seven-membered rings fused with aromatic moiety has drawn the synthetic interest of many groups. A new concise route to the key intermediate for isoindolobezazepine alkaloids, lennoxamine and chilenine, was developed through intramolecular Heck reaction of benzamide



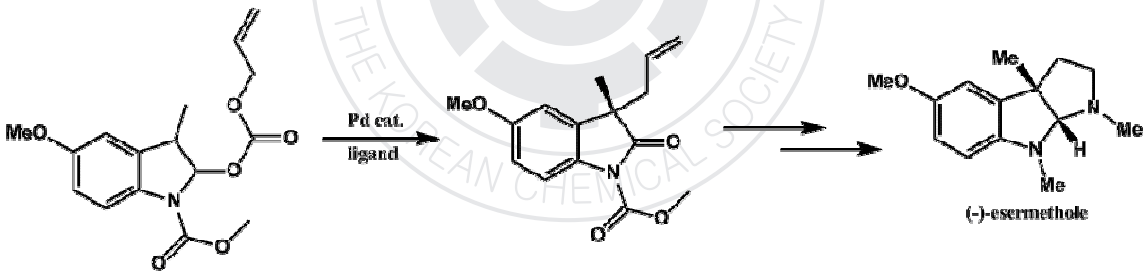
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-79**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Intramelecular asymmetry allylation for alkaloid synthesis

이승수, 박지혜, 김건철

충남대 화학과

The intramolecular allylation to produce 3,3-disubstituted oxindoles for the synthesis of esermethole is reported. Palladium-catalyzed decarboxylative asymmetric allylation of allyl enol carbonates as a highly chemo-, regio-, and enantioselective process for the synthesis of carbonyl intermediate for mesembrane bearing a quaternary α-stereogenic center has been also investigated in detail.



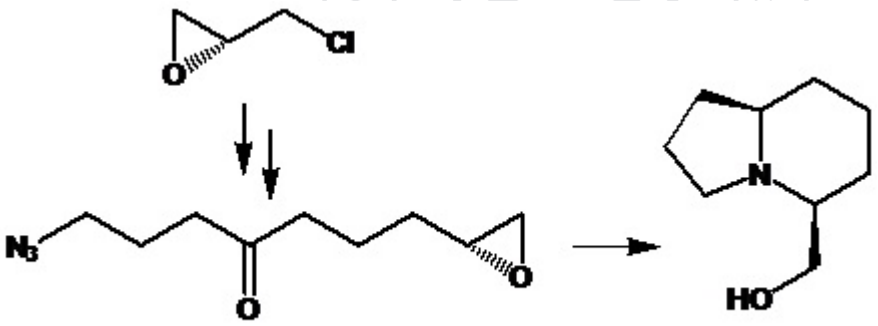
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-80**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthetic study of Indolizidine alkaloid

김민혜, 김건철

충남대 화학과

The azabicyclic ring skeleton is an important structural subunit present in numerous biologically active natural product. In this family, indolizidine alkaloids are the most important class of compounds known for their wide range of pharmaceutical application. Owing to their wide variety of biological activity, the indolizidine alkaloids have attracted much attention from synthetic chemists.In this research, we studied efficient synthetic method for 5-hydroxyazacyclic compound.



일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-81**

발표분야: 유기화학

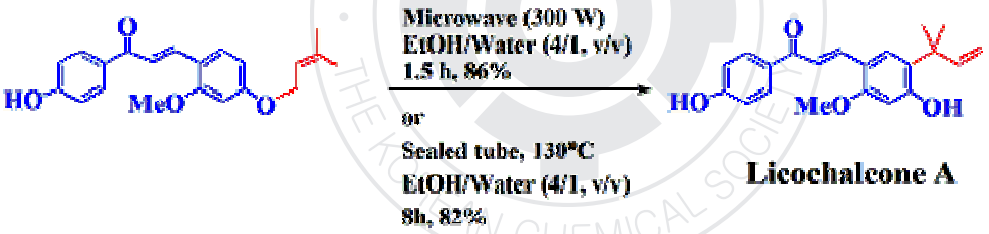
발표종류: 포스터, 발표일시: 목 10:30~12:30

Concise Synthesis of Licochalcone A through Water-Accelerated[3,3]-Sigmatropic Rearrangement of Aryl Prenyl Ether

전제호, *전종갑

*한림대 천연의약연구소 *한림대 화학과*

[3,3]-Sigmatropic rearrangement through MW irradiation or sealed tube reaction in EtOH/water co-solvent system yielded aryl prenyl ether to Licochalcone A with high yield.



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장소: 대구엑스코
발표코드: **ORGN.P-82**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

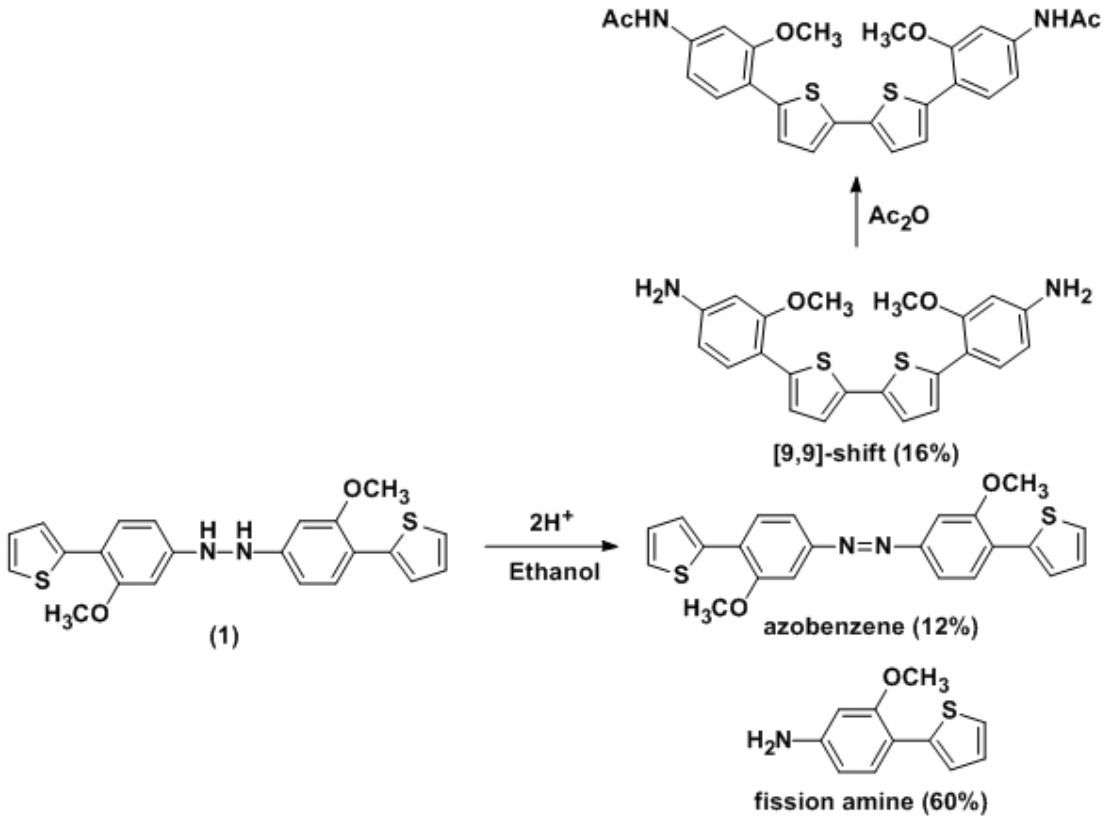
Acid-catalyzed benzidine rearrangement of bis[3-methoxy-4-(2-thienyl)phenyl]diazane. An example of [9,9]-sigmatropic shift

정동훈, 박균하

충남대 화학과

Bis[3-methoxy-4-(2-thienyl)phenyl]diazane (1) was prepared from bis[3-methoxy-4-(2-thienyl)phenyl]diazene and was set to acid-catalyzed benzidine rearrangement in ethanol solution. Product analysis showed that the rearrangement proceeded by [9,9]-sigmatropic shift together with disproportionation. The structures of products were determined by conventional spectroscopic data such as ^{1}H NMR, IR, elementary analysis and LC/MS. In paticular, identification of the structure of rearrangement product was made possible by acetylation. Futher we were able to determine the ratio of products quantatively as [9,9]-sigmatropic shift product (16%) and disproportionation in (72%).

Scheme



THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-83**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

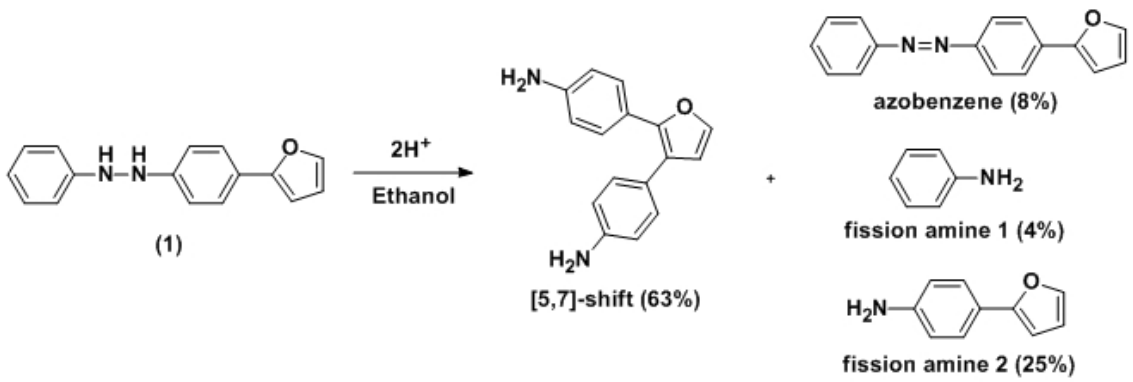
Acid-catalyzed benzidine rearrangement of [4-(2-furyl)phenyl](phenyl)diazane. An first example of [5,7]-sigmatropic shift

정동훈, 박균하

충남대 화학과

[4-(2-Furyl)phenyl](phenyl)diazane (1) was prepared by reduction of corresponding [4-(2-furyl)phenyl](phenyl)diazene in aqueous acetone solution with the use of ammonium chloride and zinc powder. The freshly prepared hydrazo (1) was subjected to acid-catalyzed benzidine rearrangement and we were able to determine the structures of the rearrangement products and their yields quantitatively based on the ^{1}H HMR spectra as shown in the scheme, that is, [5,7]-sigmatropic shift and disproportionation in 63% and 37% respectively. This [5,7]-shift provides first example in the benzidine type rearrangement.

Scheme



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-84**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

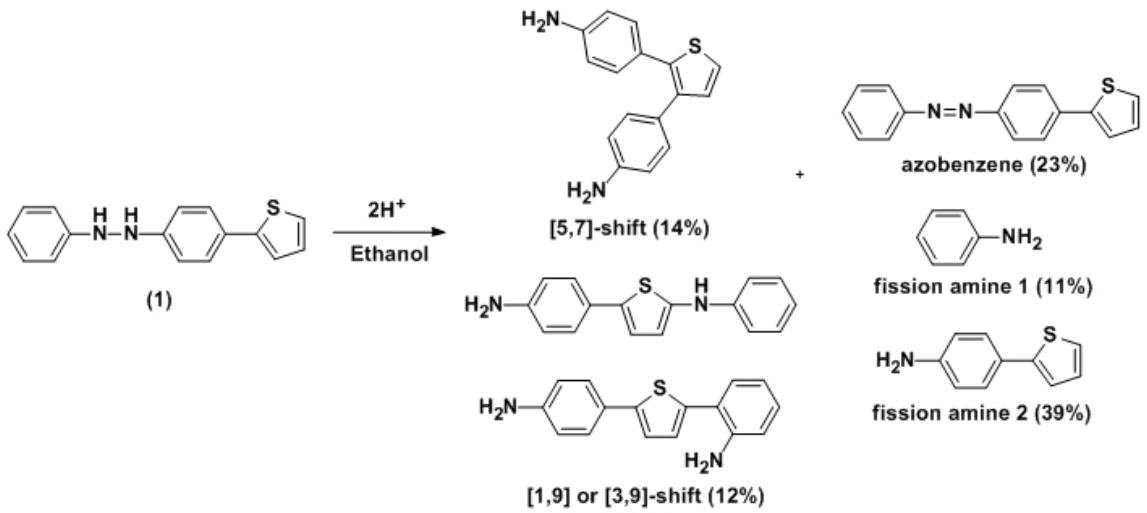
Acid-catalyzed benzidine rearrangement of [4-(2-thienyl)phenyl](phenyl)diazane. An example of [5,7]-sigmatropic shift and [1,9] or [3,9]-shift

정동훈, 박균하

충남대 화학과

[4-(2-Thienyl)phenyl](phenyl)diazane (1) prepared by reduction of corresponding [4-(2-thienyl)phenyl](phenyl)diazene was subjected to acid-catalyzed benzidine rearrangement. After work-up, we isolated and were able to determine the structure of the rearrangement product. Based on these findings the benzidine rearrangement of (1) was shown to follow [5,7]-shift (14%), [1,9] or [3,9]-shift (12%). Beside this rearrangement product, we found out that disproportionation also proceeded to give azo and fission amine (73%) as shown in the scheme. This [5,7]-shift provides second example in the benzidine type rearrangement. But to our knowledge to our [1,9] or [3,9]-shift provides first example.

Scheme



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-85**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Ratiometric fluorescent determination of Zn(II): A new class of tripodal receptor using mixed imine and amide linkages

김민정, 장두옥

연세대 화학과

We synthesized a novel receptor with a unique combination of sp2 nitrogen (-CH=N-) and carbonyl groups from amide linkages. These two moieties are judiciously incorporated into the receptor design such that these sites simultaneous binding a metal ion may generate a stable five membered ring. The receptor has been used to selectively detect Zn2+ through changes in the fluorescence spectra. Upon Zn 2+ binding with the receptor, the fluorescence band shifted to enhance fluorescence intensity , allowing ratiometric determination of Zn2+ concentration.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-86**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Organocatalytic enantioselective indium- mediated allylation of α,β-unsaturated hydrazones

김성준, 장두옥

연세대 화학과

A facile, highly isomeric ratio and highly enantioselective indium-mediated allylation of α,β-unsaturated hydrazones using cinchona alkaloid derivatives is descibed. We have developed an enantioselective indium-mediat ed allylation of α,β-unsaturated hydrazones for the preparation of enantioenriched homoallylic amines in the presence of a chiral salt. Addition reactions of allyl halides to various aldehyde and ketone derived α,β-unsaturated hydrazones were performed, affording the addition adducts in high chemical yields with high enantioselectivity.

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장소: 대구엑스코
발표코드: **ORGN.P-87**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Organocatalytic highly enantioselective al kylation and allylation of N-benzoyl hydrazones using primary alkyl halides and trialkylboranes

천지훈, 장두옥

연세대 화학과

We have developed a highly enantioselective alkylation and allylation of N -benzoyl hydrazones using primary alkyl halides/trialkylboranes and triallylborane in the presence of a chiral salt. Addition reactions of primary alkyl halides to various N-benzoyl hydrazones of aldehydes were performed , affording the addition adducts in high chemical yields with high enantioselectivity. We also developed a highly enantioselective allylation using triallylborane in the presence of a chiral salt.

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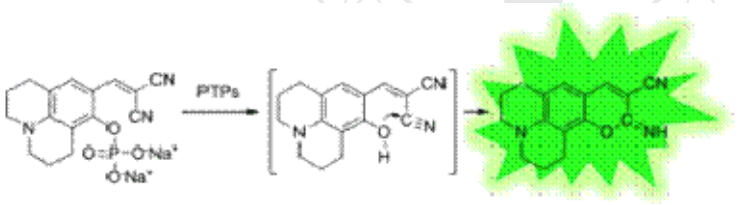
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

An Iminocoumarin-Based Fluorescent Probe for the Selective Detection of Dual-Specific Protein Tyrosine Phosphatases

김태일

단국대 화학과 유기화학전공

Protein tyrosine phosphatases(PTP) activity is revealed to associate with several human diseases, such as cancer, diabetes, and autoimmune disorders. A fluorescent probe for monitoring the activity of dual-specific PTPs has been developed. Herein, we present the design, synthesis, and application of a fluorescent probe for the detection of PTP activity with high sensitivity and selectivity and low background signal.



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발표코드: **ORGN.P-89**
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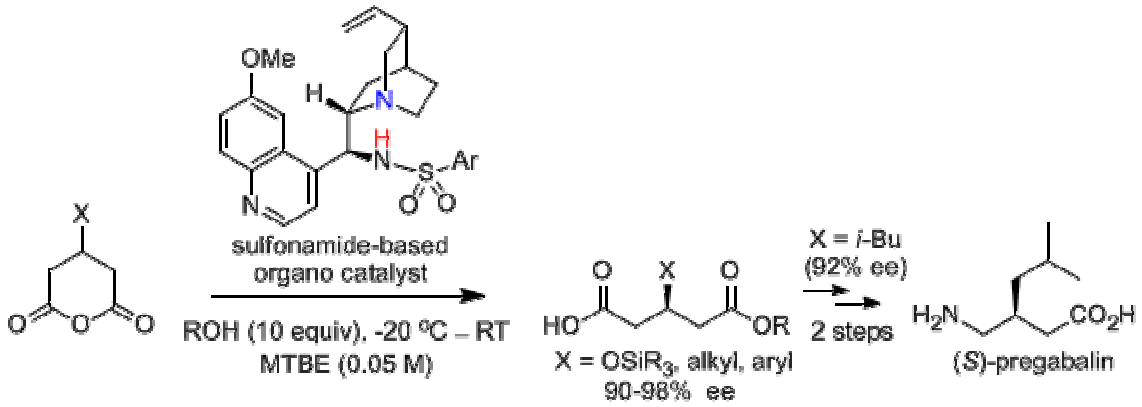
발표종류: 포스터, 발표일시: 목 10:30~12:30

Enantioselective Alcoholysis of meso Glutaric Anhydrides Catalyzed by Cinchona-based Sulfonamide Catalysts

박상은, 오중석, **Surajit Some**, *남은혜, 장형빈, 김대영, 송충의

*성균관대 화학과 *성균관대 물리협동융합과정*

We report the alcoholytic desymmetrization of a variety of meso-glutaric anhydrides with unprecedentedly high enantioselectivity using self-association free cinchona-based sulfonamide catalysts. Alcohols other than methanol were effective nucleophiles in the desymmetrization reaction and also provided excellent enantiomeric excesses (92-98% ee). DFT computational studies provide detailed insight into the observed sense of enantioselectivity. Moreover, detailed experimental studies and single crystal X-ray analysis confirmed that these bifunctional organocatalysts 3 do not form H-bonded self-aggregates in both solution and solid state. In addition, the synthetic utility of this methodology was demonstrated in the synthesis of pharmaceutically important γ-amino acids such as (S)-pregabalin. Of the many asymmetric syntheses of enantiomerically pure (S)-pregabalin reported to date, our synthesis requires the least number of and simplest steps.



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장소: 대구엑스코
발표코드: **ORGN.P-90**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

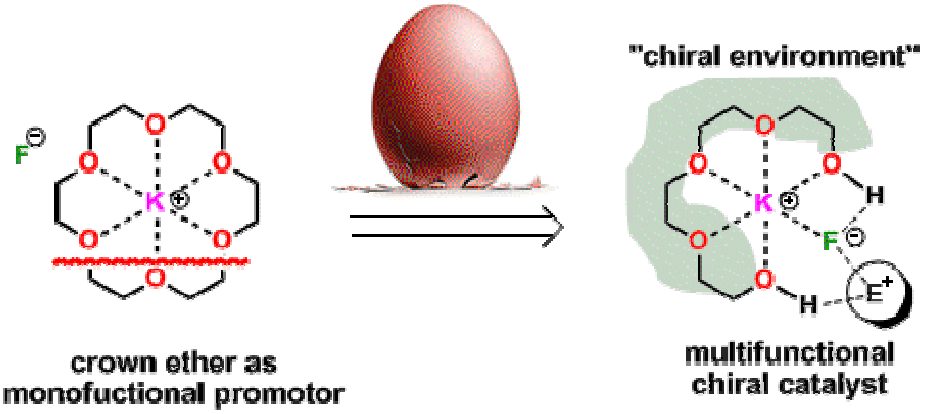
Chiral Bis-terminal Hydroxyl Polyethers as New Structural Motif for Chiral Anion Generator: Application to Catalytic Desilylative Kinetic Resolution of Silyl-Protected Secondary Alcohols

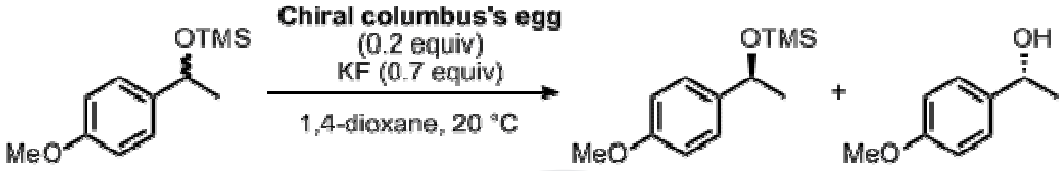
yanhailong, 장형빈, *배한용, 송충의

*성균관대 화학과 *성균관대 자연과학부 화학과*

We report a new structural motif for chiral anion generator, composed of a bis-terminal hydroxyl polyether bearing a 3,3´-halogen-substituted chiral BINOL and its successful application as a multifunctional catalyst for the enantioselective desilylative kinetic resolution of silyl-protected racemic secondary alcohols with KF, which constitutes a conceptually new approach to the production of optically active silyl-protected secondary alcohols. An array of O-silyl-protected racemic alcohols was kinetically resolved with good to excellent selectivity factors (s = up to 30, i.e., >97% ee for the remaining substrate at 56% conversion). The single crystal X-ray structure of the complex of the catalyst and KF provides detailed and interesting insight into the origin of the catalytic activity and stereoselectivity.

Columbus's egg





selectivity factor = 30
(97.3% ee at 56% conversion)

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Physical Properties of 7-(4,6-Disubstituted-1,3,5-Triazin-2-yl)aminocoumarin Derivatives as the Fluorescent Brightners

임중철, 이지연, 강용한

한양대 응용화학과

Coumarin derivatives are used as the Fluorescent Brightners effectively for animal textile materials, synthetic polyamide, and acetate fibers. Various 7-(4,6-disubstituted-1,3,5-triazin- 2-yl)aminocoumarin derivatives have been prepared from the reaction of 7-aminocoumarin derivative with cyanuric chloride (1), followed by nucleophilic substitution reaction of various amines with the remained 2- and 4-chloride on triazine moiety. Synthetic details and the whitness and fastness of the newly prepared compounds will be discussed.

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Synthesis and Physical Properties of Unsymmetrically substituted Bis(triazinylamino)stilbenes as the Fluorescent Whitening Agents

박진기, *전양준, 강용한

*한양대 응용화학과 *한양대 과학기술대학 응용화학전공*

Disodium 4,4'-bis(triazinylamino)stilbene-2,2'-disulfonate derivatives are most widely used as the fluorescent brighteners for the whitening of both cotton and wool. A planner molecular structure with conjugated double bonds, electron–donating, and withdrawing groups are necessary for the fluorescent brighteners to show the high fluorescence activity. The key intermediate for the synthesis of unsymmetrically substituted bis(triazinylamino)stilbenes, 4-(1,3,5-triazin-2-yl)amino-4'-aminostilbene-2,2'-disulfonates derivatives, were prepared from 4-(1,3,5-triazin-2-yl)amino-4'-nitrostilbene-2,2'-disulfonates by using the tin chloride as the reducing agent. Synthetic details and the whitness and fastness of the newly prepared compounds will be discussed.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Physical Properties of 2,6-disubstituted-4-(1,3-thiazol-2-yl)amino-[1,3,5]-triazine derivatives as inhibitors of MARK

이혜미, 강용한

한양대 응용화학과

4-(1,3-Thiazol-2-yl)aminopyrimidine derivatives inhibit microtubule affinity regulating kinase(MARK) and therefore find use in treatment of neurodegenerative diseases associated with hyperphosphorylation of tau. In this research, 2,6-disubstituted-4-(1,3-thiazol-2-yl)amino-[1,3,5]-triazine derivatives were synthesized as inhibitors of MARK. Synthetic details and the physical properties will be discussed.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of the Olefin-linked Fluorescent Dye-labled Uridine Derivatives

안정희, *이정선, 강용한

*한양대 응용화학과 *한양대 과학기술대학 응용화학과*

In the course of our work, we synthesized the olefin-linked fluorescent dye-labled 2‘-deoxyuridine derivatives by using the thymidine as a starting material. The oxidation of methyl group of thymidine, followed by the reaction with malonic acid in pyridine provided the 2‘-deoxyuridine containing the olefin-linker at 5-position. The fluorescein derivatives were used as the fluorescent dyes. Synthetic details and the physical properties will be discussed.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Dramatic Change of Reactivity upon Addition of Water in Photolysis of 2-Hydroxy-4,6-dimethylphenacyl Benzoate

박봉서, 임범희

동국대 화학과

Irradiation of ortho-hydroxyphenacyl benzoate (OHPB) results in formation of chromanone. As our continuing efforts to elucidate structural factors of photochemical behaviors of organic compounds, we have studied photochemistry of derivatives of OHPB containing a methyl group at the other ortho position. Accordingly, 2-hydroxy-4,6-dimethyl phenacyl benzoate was prepared and its photochemical behavior was investigated in detail. In dry solvents such as anhydrous acetonitrile or acetone, indanone was formed from a dienol intermediate via hydrogen abstraction from o-methyl group in triplet excited state. On the other hand, when a small amount of water was added to the same solvents, a dramatic change of photoproduct to chromanone and isochromanone was observed. The origin of the product selectivity will be described in detail.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Photochemistry of Ortho-alkylphenacyl Phenylglyoxalates : Mechanistic Implication into Photochemistry of Ortho-alkylphenacyl Carboxylates

박봉서, 김설희

동국대 화학과

Recently we have reported a unique solvent effect on product selectivity in photolysis of ortho-alkylacetophenones containing a leaving group at alpha position to the carbonyl. In nonpolar solvents such as benzene, corresponding indanones were formed as major products via enol intermediates formed from photoinduced hydrogen abstraction reaction. In hydrogen bond donor solvents such as methanol, however, the major products became benzocyclobutenols which were well known photoproducts of o-alkylphenyl ketones. The mechanistic reasoning behind such selectivity has been revealed in our recent investigation of photochemistry of the title compound. Our results will be presented in detail.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **ORGN.P-97**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

$FeCl_3$-Catalyzed Synthesis of 2-Methyl-4-amino-1,2,3,4-tetrahydroquinoline Derivatives by the Imino Diels-Alder Reaction

CHEN YE, 이용록

영남대 화학공학부

We describe herein an efficient and simple method for the synthesis of 2-methyl-4-amino-1,2,3,4-tetrahydroquinoline derivatives starting from a variety of anilines with N-vinyl pyrrolindine-2-one in the presence of $FeCl_3$.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Metathesis-Based Synthesis of Cyclic Peptoids

sharaf nawaz khan, *Robert H. Grubbs, 권용억

*이화여대 화학.나노과학과 *Division of Chemistry and Chemical Engineering, California Institute of Technology*

Peptides are an attractive class of molecules which contain protein-binding properties. However, they have several undesirable drawbacks including sensitivity to proteases, limited cell permeability and poor bioavailability. Thus, there have been increasing needs for new peptidomimetics with improved pharmacokinetic characteristics. Among them, peptoids, N-alkylated glycine oligomers where side chains are directly attached to nitrogen atom rather than ´ -carbon of peptide, possess many advantages over peptides. In addition, cyclic peptides and depsipeptides have received a great deal of attention because of their challenging chemical synthesis and numerous interesting bioactivities including antibiotic activities, enzymatic inhibitory activities and therapeutic properties. Moreover, cyclic molecules might be presumed to bind more tightly to their protein targets due to their more restricted conformational flexibility in some cases. The limitations of peptides, along with the fascinating properties of cyclic molecules and peptoids, have led to the development of cyclic peptoids. For the macrocyclozation of peptoids on solid-phase, we employed olefin metathesis, more exactly, ring-closing metathesis. We have successfully synthesized cyclic peptoids through solid-phase RCM, regardless of the ring sizes for 16- to 25-membered cyclic peptoids both under microwave conditions and at 40 oC. HG2 was a better catalyst than G1 and G2. The cyclization facilitated easily with 3-buten-1-amine over allylamine. This systematic study in to the use of solid-phase RCM for the synthesis of cyclic peptoids provides a particularly valuable tool for easy access to the molecular sources of cyclic compounds and the rapid generation of cyclic peptoid libraries, which are currently under way.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Ready Access to Glycopeptoids as Glycopeptide Mimetics

조수경, 권용억

이화여대 화학.나노과학과

It is essential to investigate the biological functions of each protein in the post-genome era. It is also well known that proteins are modified by post-translational modification such as glycosylation and phosphorylation in higher organisms, resulting in the exponential expansion of protein structures and functions. In particular, glycoproteins are involved in various biological phenomena including cell-cell interaction, signaling, immune recognition and developmental regulation. Despite of these crucial functions of glycoproteins, the systematic studies of the effects of protein glycosylation have been limited due to the heterogeneity and structural complexity of carbohydrates. In order to access glycopeptides and glycoproteins of defined structure, various chemical, enzymatic and genetic approaches have been developed. In this regard, we also envisioned to develop chemical tools for glycomics. As glycopeptide mimetics, glycopeptoids were adopted because peptoids have many advantages over peptides, including easy synthesis of libraries, a myriad of chemical diversity, proteolytic resistance and improved cell permeability. For the construction of glycopeptoid libraries, O-linked and N-linked glycopeptoids were synthesized on solid-phase using 'submonomer strategy' with many commercially available primary amines and synthetically prepared sugar amines. Especially, diastereomeric sugar monomers were strategically differentiated by using different amine linkers, resulting in successful sequencing by tandem mass spectrometry (MS/MS). Glycopeptoids should be useful chemical tools for glycomics, chemical biology, drug development and diagnostic studies of diseases.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Highly efficient blue emitting materials based on N,N-diphenyl aminofluorene styryl derivatives

주혜진, 이금희, *김영관, 윤승수

*성균관대 화학과 *홍익대 기초과학과*

Organic light emitting diodes (OLEDs) have been considered as the next generation displays because of its great potential in full color flat-panel display. However, blue emitting materials have some problems involved color purity, efficiency, and thermal stability. These are closely related with efficiency of devices, thus it is important to develop better blue emitting materials. In this study, we designed, synthesized, and characterized more efficient blue-emitting materials which have a common structure 9,9-diethyl-N,N-diphenyl-7-styryl-9H-fluoren-2-amine. Among those materials, the derivative with benzothiophenyl group shows the maximum luminance of 10230 cd/m^2 at 10 V, the luminous efficiency of 12.8 cd/A at 20 mA/cm^2, power efficiency of 4.36 lm/W at 20 mA/cm^2 and CIE x,y coordinates of (x = 0.155, y = 0.200) at 10 V. Particularly, the derivative with phenoxybiphenyl group shows the best CIE x,y coordinates of (x = 0.147, y = 0.130) at 10 V, the maximum luminance of 6415 cd/m^2 at 10 V, the luminous efficiency of 8.47 cd/A at 20 mA/cm^2, and power efficiency of 3.67 lm/W at 20 mA/cm^2

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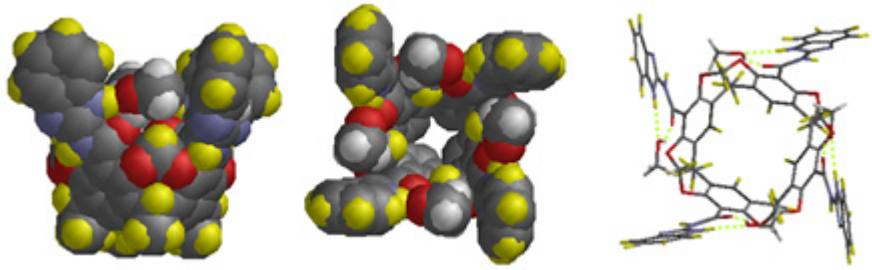
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Alcohol-mediated self-folding amidobenzimidazole-cavitand

박연실, 서성종, 백경수

숭실대 화학과

Resorcin[4]arene-based cavitand bearing four amidobenzimidazole moieties on the upper can fold into vase conformer by hydrogen bonds mediated with an alcohol molecules between amide C=O and benzimidazole N-H proton. Consequently a narrow and deep cavity is formed and stabilized, and the protons of the benzene ring in the NH side of benzimidazole moieties perpendicularly contact to neighboring benzimidazole moiety, which can be confirmed by ^{1}H NMR spectrum ($CD_3OD/CDCl_3$ =1:5). This self-folding cavitand shown below forms kinetically stable complexes with normal alkanes, from pentane through to octane. Their conformations and binding properties were studied by ^{1}H NMR and 2D NMR.



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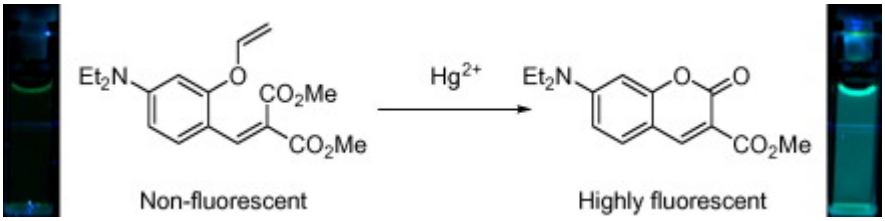
장소: 대구엑스코
발표코드: **ORGN.P-102**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

A Novel Fluorescent Chemodosimeter That Selectively Responds to Inorganic Mercury Species

조용석

포항공과대 화학과

Yong-Suk Cho and Kyo Han Ahn*Department of Chemistry and Center for Electro-Photo Behaviors in Advanced Molecular Systems, POSTECH, Pohang, Republic of Korea, 790-784ahn@postech.ac.krMercury is a highly poisonous element and exists as elemental, inorganic, and organic mercury forms. Contaminated living species, soil and water typically contain inorganic and organic mercury forms.[1]Fluorescent probes can be categorized to two types based on the sensing mechanism: one based on metal coordination and the other based on a chemical reaction.[2] The reaction-based fluorescent sensing approach for inorganic mercury species has attracted sudden research interest recently, plausibly owing to the high selectivity obtainable. We devised a reaction-based fluorescent sensing system from a fluorescein that senses not only organic mercury but also inorganic mercury among various other metal species examined.[2] In this presentation, we have investigated other vinyl ether systems that may discriminate methylmercury from inorganic mercury species or vice versa. The sensing process involves a mercury ion-promoted hydrolysis (oxymercuration reaction) followed by cyclization, which leads to a fluorescent coumarin, in the presence of inorganic mercury species among various other metal species.[2]1. ATSDR 2005. ToxProfiles: Mercury: Atlanta, GA, U.S. Department of Health and HumanServices.2. Nolan, E. M.; Lippard, S. J. Chem. Rev. 2008, 108, 3443.3. M. Santra, D. W. Ryu, A. Chatterjee, S. K. Ko, Injae Shin, K. H. Ahn, Chem, Commun. 2009, 2115.4. Cho, Y.-S.; Ahn, K. H. Tetrahedron. Lett. 2010, 51, 3852.



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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

The synthesis of poly(lactic acid) oligomers using solid-phase synthesis

김성호, *이혁

*한국화학연구원 의약화학 *한국화학연구원 신약연구단*

Poly(lactic acid) has attracted a highly attention due to its biodegradable and biorenewable properties. Wide usages of poly(lactic acid) have been found from biomedical application to biodegradable packaging. Recently the interest in the synthesis of poly(lactic acid) oligomers and their physical properties are also increased for the better understanding of poly(lactic acid) . However, synthetic strategy for poly(lactic acid) oligomers were still limited. Facile synthesis of poly(lactic acid) oligomers using solid-phase synthesis is described. Without separations, the desired poly(lactic acid) oligomer was easily synthesized under mild condition in high yields. Also by controling the reaction order of (R)- or (S)-lactic acid, diverse poly(lactic acid) oligomers were produced. Also the application of the poly(lactic acid) oligomers were attempted.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

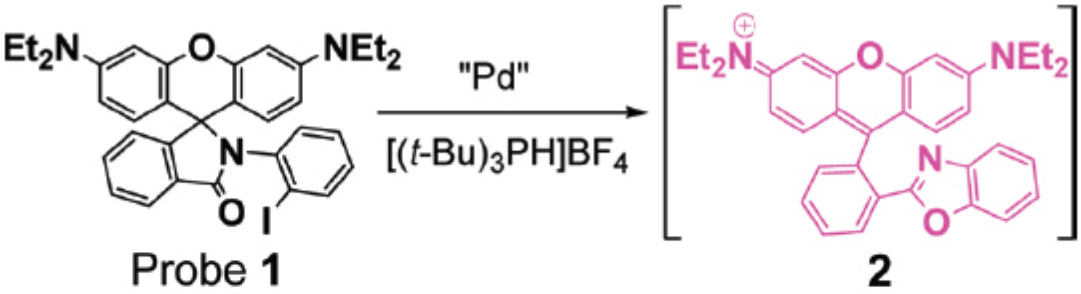
Catalytic Reaction-based Fluorescent and Chromogenic Sensing of Palladium Species

전미은

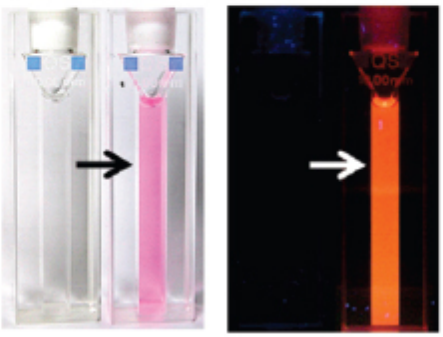
포항공과대 화학과

Palladium catalyzed cross-coupling reaction has found an important place in modern synthetic protocols because it can perform to make difficult covalent bond in medicine and materials. However, even after purification, residual palladium is often found in the final product, which may be a health hazard. For that reason, easy detection of palladium species is an important goal.[1] Along with our efforts to develop efficient molecular probes based on organic reactions,[2] we have developed a simple yet efficient detection method for palladium species based on a molecular sensing system that undergoes a palladium catalyzed oxidative addition.[3] A rhodamine B derivative thus developed undergoes the catalytic process triggered by palladium insertion and gives both turn-on fluorescence and color changes. The catalytic ring-opening process is specific toward palladium species such as PdCl2 or Pd2dba3 in the presence of [(t-Bu)3PH]BF4] at 85 °C, among various metal chloride species examined. A usefulness of the sensing system is demonstrated by determining the residual palladium contents in a purified sample prepared through a palladium-catalyzed reaction. This is the first reaction-based sensing system for palladium species that gives both the turn-on fluorescence and color changes.

Reference:1. Song, F.; Garner, A. L.; Koide, K. J. Am. Chem. Soc. 2007, 129, 12354.2. (a) Ryu, D.; Park, E.; Kim, D. S.; Yan, S.; Lee, J. Y.; Chang, B. Y.; Ahn, K. H. J. Am. Chem. Soc. 2008, 130, 2394. (b) Chatterjee, A.; Santra, M.; Won, N. Y.; Kim, S. J.; Kim, J. K.; Kim, S. B.; Ahn, K. H. J. Am. Chem. Soc. 2009, 131, 2040. (c) Santra, M.; Ryu, D.; Chatterjee, A.; Ko, S. K.; Shin I.; Ahn, K. H. Chem. Commun. 2009, 2115. (d) Egorova, O. A.; Seo, H.; Chatterjee, A.; Ahn, K. H. Org. Lett. 2010, 12, 401. (e) Santra, M.; Ko. S.-K.; Shin, I.; Ahn, K. H. Chem. Commun. 2010, 46, 3964.3. Jun, M. E.; Ahn, K. H. Org. Lett. 2010, 12, 2790.



Probe **1** **2**



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and biological evaluation of ^{64}Cu-TE2A-Bz-NCS-c(RGDyK) for PET imaging of tumors expressing $\alpha_v\beta_3$ integrin

DARPAN, *김정영, **박정찬, **곽원정, 왕은경, 하영수, ***안광일, **유정수

*경북대 의과학과 *한국원자력의학원 방사성의약품연구팀 **경북대 의과대학 분자의학교실 *** 한국원자력의학원 방사성의약품 개발실*

The choice of bifunctional chelator and radioisotope are crucial for successful tumor imaging using target-specific peptides. ^{64}Cu($t_{1/2}$ 12.7 h) is both a β+ and a β-emitter allowing it to be used for both imaging and radiotherapy. In order not to sacrifice any carboxylate coordination to Cu(II) ions in Cu-TE2A complex, we introduced a third orthogonal pendant arm having -NH_2 or -NCS functionality suitable for conjugation with peptides or antibody. This preparation of TE2A-NCS is highly efficient in terms of overall yield (57%) and number of synthetic steps (7) as well as facile purification compared to all route published previously involving other bifunctional chelators with NH_2/NCS linkers. The TE2A-NCS-c(RGDyK) is labeled with ^{64}Cu to greater than 95% purity and 90% yield within 10 min at 30°C. U87MG tumors were clearly visualized by ^{64}Cu-TE2A-NCS-c(RGDyK) with high signal to background ratio at 1 and 4 h postinjection. Biodistribution studies showed that the liver and kidneys were the only organs to have similar or slightly higher uptake of ^{64}Cu-TE2A-NCS-c(RGDyK) than the tumor. TE2A-NCS might be widely utilized to label many disease-specific peptide and antibody thanks to its easy conjugation with biomolecules and easy radiolabeling with ^{64}Cu(II) ions

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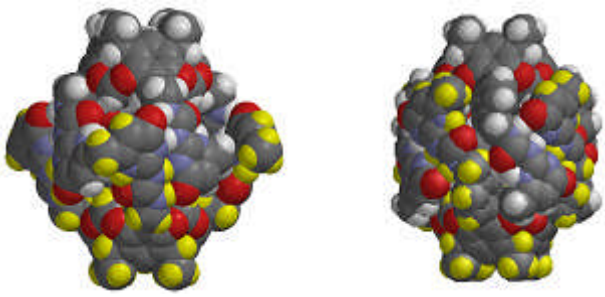
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Ureidopyrimidone molecular capsule though quadruple hydrogen bondings

서성종

숭실대 화학과

Self-assembling molecular capsules based on noncovalent interactions have attracted considerable interest due to their potentials as molecular storage, sensor, catalysts, or reaction chambers in the field of supramolecular chemistry. Resorcin[4]arene-based cavitands having four ureido-4[1H]-pyrimidone moieties on the upper rim formed stable molecular capsules in nonpolar solvents by the four quardruple intermolecular hydrogen bondings via donor-donor-acceptor-acceptor hydrogen bonding array in the 4[1H]-pyrimidone tautomer, four from each four paired ureido-4[1H]-pyrimidone, and the four intramolecular hydrogen bondings from the pyrimidine N-H group to the urea oxygen atom on each cavitand. The synthesis and versatile characteristics of this ureido-4[1H]-pyrimidone molecular capsule toward anionic, cationic, and neutral guests will be presented.



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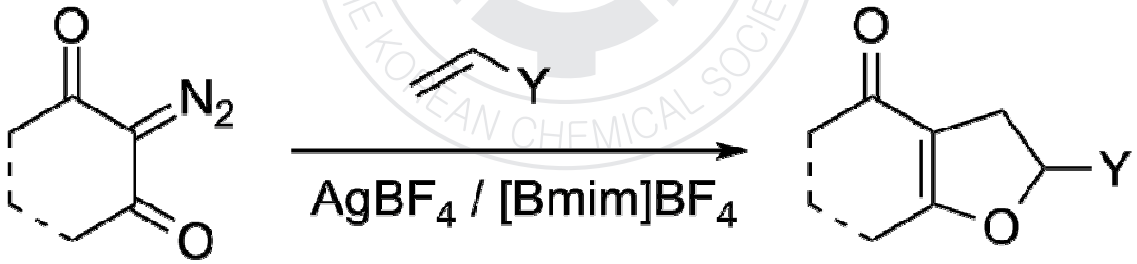
발표종류: 포스터, 발표일시: 목 10:30~12:30

Efficient Synthesis of 2,3-Dihydrofurans by $AgBF_4$/[Bmim]BF_4-Catalyzed [3+2] Cycloaddition of Cyclic Diazodicarbonyl Compounds with Olefins

하립개, 이용록

영남대 화학공학부

A novel and efficient method for the synthesis of 2,3-dihydrofurans was achieved by the reaction of cyclic diazodicarbonyl compounds with styrene and vinyl acetate. The key strategy was $AgBF_4$/[Bmim]BF_4/-catalyzed [3+2] cycloaddition reactions.



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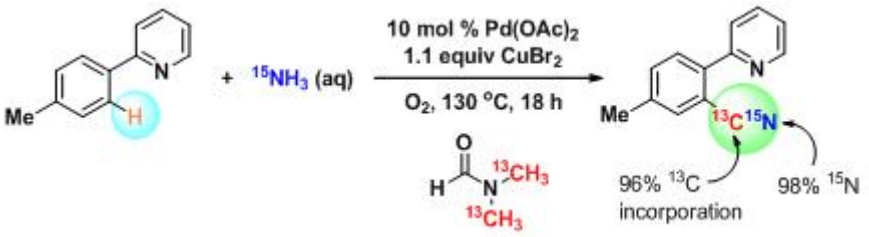
A New Combined Source of "CN" from N,N-Dimethylformamide and Ammonia in the Palladium-Catalyzed Cyanation of Aryl C–H Bonds

김진호, 장석복

KAIST 화학과

Aromatic nitriles possess versatile utilities and are indispensible not only in organic synthesis but also in chemical industry. In fact, the nitrile group is an important precursor for various functional groups such as aldehydes, amines, amidines, tetrazoles, amides, and their carboxyl derivatives. Representative methods for the preparation of organonitriles with cyanide-containing reagents are the Sandmeyer and Rosenmund-von Braun reactions. Recently, a catalytic route to aryl nitriles has been reported on the basis of the chelation-assisted C–H bond activation or metal-catalyzed cyanation of haloarenes. In those cyanation protocols, the "CN" unit is provided from metal-bound precursors of MCN (M = Cu, K, Na, Zn), TMSCN, or K3Fe(CN)6. Additionally, it can be generated in situ from nitromethane or acetone cyanohydrin. Herein, we report the first example of generating "CN" from two different, readily available precursors, ammonia and N,N-dimethylformamide (DMF). In addition, its synthetic utility is demonstrated through the Pd-catalyzed cyanation of arene C–H bonds.



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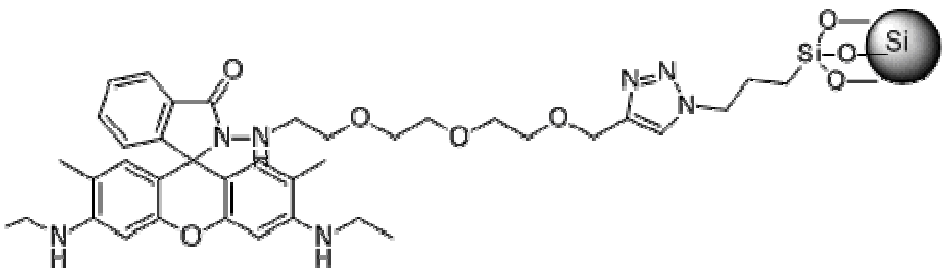
발표종류: 포스터, 발표일시: 목 10:30~12:30

Detection of acid vapors by rhodamine hydrazide immobilized on mesoporous silica

김소연, 태진성

연세대 화학과

The real-time sensing of volatile organic compounds (VOCs), such as amines, hydrocarbons, explosives, and chemical warfare agents, has been an active research area. Although much success has been achieved for the detection of VOCs by using various optical detection methods, the fluorescent probe-based sensing of VOCs still remains challenging, mainly because there are not many organic materials available which are sufficiently fluorescent in solid state and suitable for vapor detection. So we developed the chemosensor for detection of volatile acidic gases in solid state. Fluorescent and colorimetric volatile acidic gas sensor was prepared by immobilization of rhodamine hydrazide onto mesoporous silica. Upon flow of volatile acidic gases to the modified silica, the silica resulted in a color change from white to pink and fluorescent change. No significant color or fluorescent changes were observed in the response to organic gases or other volatile organic compounds(VOC). Diethyl chlorophosphate (DCP), one of model compounds used for the studies of Chemical Warfare Agent (CWA), could also be detected by using this method.



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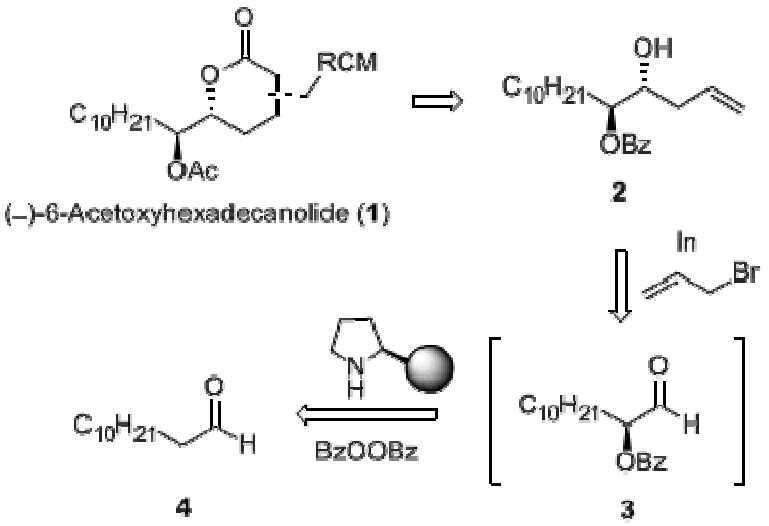
Total Synthesis of (−)-6-Acetoxy-5-hexadecanolide by Organocatalytic α-Oxygenation−Allylation−RCM Strategy

박영주, 태진성

연세대 화학과

In the past few years organocatalysis, complementing bio- and metal-catalysis, has attracted much attention and employed in numerous asymmetric synthesis. Considerable effort has also been devoted to the development of tandem reactions following the asymmetric organocatalytic reactions in one−pot operation, thereby avoiding the isolation of reaction intermediates, to synthesize diverse chiral building blocks from simple precursors. Recently, Maruoka *et al* reported an organocatalytic α-benzoyloxylation of aldehydes with benzoyl peroxide catalyzed by (*S*)-2-tritylpyrrolidine. Tandem allylation of the α-benzoyloxy aldehydes could readily generate the monoprotected 1,2-diols which could serve as the key intermediates in asymmetric synthesis. In continuation of our interest to explore tandem reactions of the organocatalytic reactions, we have developed a facile enantioselective synthesis of (−)-(5*R*,6*S*)-6-acetoxy-5-hexadecanolide (1). Organocatalytic α-benzoyloxylation of dodecyl aldehyde (4) with benzoyl peroxide catalyzed by chiral pyrrolidine followed by indium-mediated *in situ* allylation of the resulting α-benzoyloxyl aldehyde 3 afforded the monoprotected 1,2-diol 2 as shown in the retrosynthesis. Conversion of the homoallyl alcohol 2 to the corresponding acryl ester followed by ring-closing metathesis (RCM) and hydrogenation generated the benzoyloxy derivative of 1.



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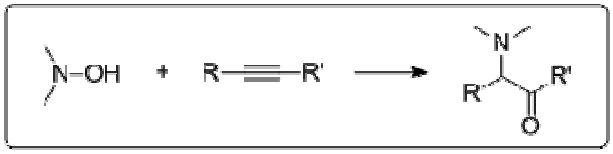
Oxygen-Transfer Reactions of N-Sulfonyl Hydroxylamines via Gold Catalysis: Synthesis of Pyrrolidinones and Nitrones

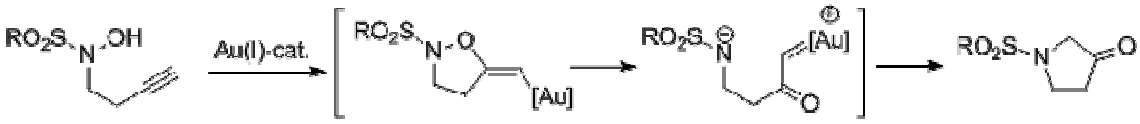
염현석, 소은수, 신승훈

한양대 화학과

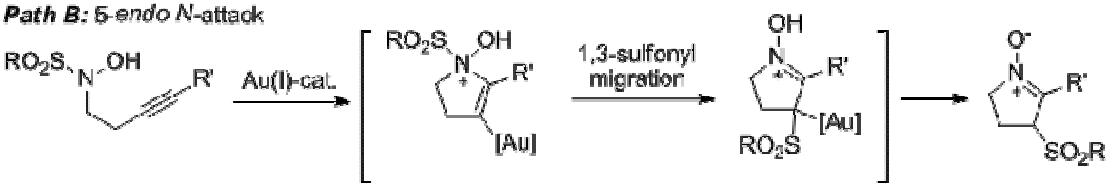
In order to increase molecular complexity of simple organic substrates, atom transfer protocols have received intense attention from a viewpoint of atom- and redox-economy. For example, various hydrogen-exchange processes enable a synthetic design that bypasses redox adjustment steps required to generate reactive functional groups for the desired C-C bond formation. On the other hand, we have reported a number of oxygen-exchange protocols from the hydroxylamine derivatives, for the in-situ generation of reactive functionality such as carbene, enolate and azomethine ylide.We projected that the addition of R_2N-OH onto alkyne will lead to alpha-amino carbonyl compounds that constitute a fundamental organic building block. We realized this concept in an intramolecular fashion using alkyne tethered N-sulfonyl hydroxylamines. Depending on the alkynyl substituents, the reaction follows two distinct manifold, namely 3-pyrrolidinones and nitrones. The details of this chemistry will be presented.



Path A: *5-exo O-attack*



Path B: *5-endo N-attack*



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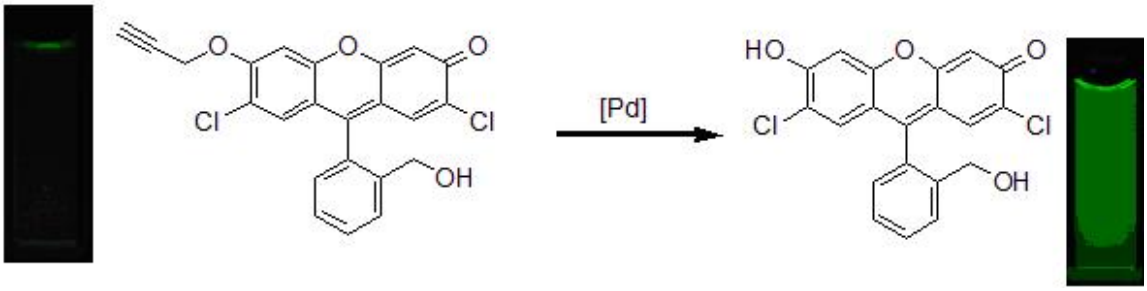
A Chemodosimeter Approach to Fluorescent Sensing and Imaging of Palladium Species

Mithun Santra

포항공과대 화학과

In chemical transformations, palladium plays a key role as a catalyst in the synthesis of various molecules including drugs.[1] It is also widely used to prepare dental materials, electric equipments, automobile exhaust catalysts, and fine jewellery. However, the palladium metal complexes influence our health and environment in an adverse way because palladium ions can bind to thiol-containing amino acids, proteins (casein, silk fibroin, and many enzymes), DNA or other macromolecules (vitamin B6) and thereby may disturb a variety of cellular processes.[1] Therefore, it is desirable to develop efficient methods for detecting the presence of palladium species. Palladium complexes exhibit oxidation states of 0, +2, and +4 as in the typical cases of Pd(PPh3)4, PdCl2 and PdCl62– respectively. Among all the palladium species, PdCl2 is the most toxic one. We have devised a fluorescein-based propargyl ether derivative 1 which is found to detect palladium species selectively at room temperature and shows a turn-on type fluorescent response. Here the propargyl ether derivative undergoes palladium catalyzed hydration pathway.[2, 3] Significantly, the probe senses palladium species in all the typical oxidation states (0, +2, and +4) without adding any additional reagents. With this probe we have monitored the accumulated palladium species in living organisms. The results demonstrate for the first time that probe 1 is potentially useful for monitoring palladium species in living organisms. References (1) International Programme on Chemical Safety. Palladium; Environmental Health Criteria Series 226; World Health Organization: Geneva, 2002. (2) Pal, M.; Parasuraman, K.; Yeleswarapu, K. R. Org. Lett. 2003, 5, 349.(3) Sarin, G. S. Tetrahedron Lett. 1993, 34, 6309. (4) Domaille, W. D.; Que, L. E.; Chang, J. C. Nat. Chem. Biol. 2008, 4, 168.(5) Lichtman, J. W.; & Conchello, J. A. Nat. Methods. 2005, 2, 910.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

A novel synthesis of TE2A and its use as a potential bifunctional chelator

AJIT DALE, *DARPAN, **김정영, *박정찬, *곽원정, ***안광일, *유정수

*경북대 의과학과 *경북대 의과대학 분자의학교실 **한국원자력의학원 방사성의약품연구팀 ***한국원자력의학원 방사성의약품 개발실*

Interest in the synthesis and use of polyazamacrocycle derivatives as a bifunctional chelator has increased tremendously over last few decades, due to their potential application in diagnostic and therapeutic medicine. Their prime importance as a bifunctional chelator is to hold radiometals strongly in a biological environment. Recently, TE2A was found to make kinetically more stable Cu(II) complexes than TETA. Here we report a new synthetic route for TE2A. First step of TE2A synthesis was the formation of bisaminal compound from cyclam. The regioselective trans-alkyl disubstitution of bisaminal was done with benzyl bromoacetate, followed by successive deprotection of the methylene bridge and benzyl group to give TE2A in a salt-free form with an overall yield of 74 %. TE2A was quantitatively radiolabeled for microPET imaging with ^{64}Cu using $^{64}CuCl_2$ in 0.1 M NH_4OAc buffer solution at pH 6.5-6.8. Its imaging result clearly showed that the complexed compound was excreted rapidly from the body via urinary and hepatobiliary system. TE2A was further conjugated with c(RGDyK) peptide through one carboxylate group using the standard EDC/SNHS conjugation method. The TE2A-c(RGDyK) conjugate was then radiolabeled with ^{64}Cu in 94 % yield in 0.1 M NaOAc buffer solution at pH 8. We report the novel synthetic method for TE2A in salt-free form, overcoming serious drawbacks of the previous methods. TE2A showed a good radiolabeling yield with $^{64}Cu(II)$ ions. TE2A was also conjugated with the cyclic RGDyK peptide and the TE2A-c(RGDyK) conjugate was successfully radiolabeled with ^{64}Cu in high yield, demonstrating its potential as a bifunctional chelate without any further structural modification.

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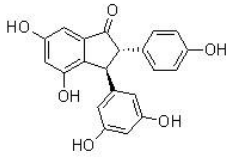
Stereoselective Total Synthesis of (+)-Pauciflorol F via Palladium-Catalyzed *α*-Arylation of 1-Indanone

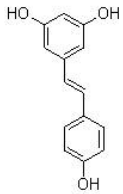
이봉향, *최영록, 신승훈, **허정녕

*한양대 화학과 *고려대 화학과 **한국화학연구원 신약연구단*

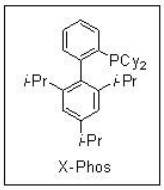
Pauciflorol F (1) belongs to a large family of polyphenolic natural products including resveratrol (2) and its derivatives, which receive much attention due to interesting biological activities such as anticancer, antibacterial, and anti-HIV. Our approach centers on the strategic employment of stereoselective *α*-arylation of 1-indanone with aryl bromide under Pd-catalyzed conditions. For example, reaction of 1-indanone 3 with 4-bromoanisole in the presence of $Pd(OAc)_2$ and X-phos provides *trans* indanone 4, the precursor of pauciflorol F, in 90% yield with high stereoselectivity (*trans* : *cis* = > 25 : 1). Synthetic efforts toward total synthesis of (+)-pauciflorol F will be discussed.

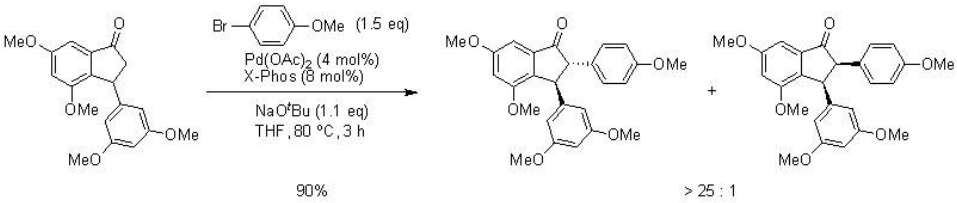


Paucilflorol F (1)



Resveratrol (2)





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Efficient One-Pot Synthesis of α-Chloroenones with β-Carbonates and β-Carbamates

SOMAI MAGAR KRISHNA, 이용록

영남대 화학공학부

An efficient synthesis of enones with α-chloro and β-carbonates or β-carbamates was achieved by rhodium(II) catalyzed reaction of cyclic diazodicarbonyl compounds with a variety of chloroformates and carbamyl chlorides in moderate yields. These reactions provide a useful and rapid entry to β-substituted α-haloenones.

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Efficient Synthesis of Stemofuran A and Its Derivatives

NEUPANE PRATIK, 이용록, *이희진

*영남대 화학공학부 *거림테크(주) 부설연구소*

Stemofuran A and its derivatives are isolated from *Stemona collinsae*. This plant has been used in traditional Asian medical pratices for the treatment of inflammatory-related diseases. A simple and concise synthesis of stemofuran A and its derivatives will be described in this presentation.

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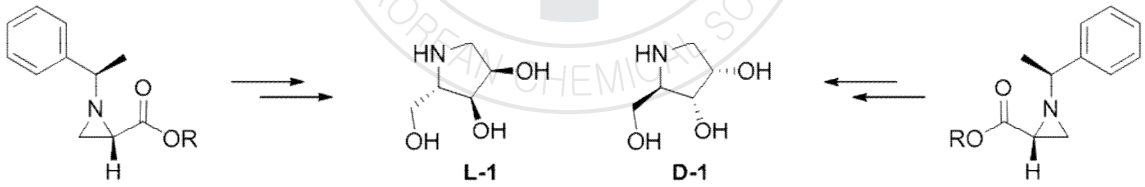
Synthesis of 1,4-Dideoxy-1,4-iminoribitol

엄희성, 하현준, *이원구

*한국외국어대 화학과 *서강대 화학과*

1,4-Dideoxy-1,4-iminoribitol, one of many polyhydroxypyrrolidine natural products with interesting biological activities, was synthesized starting from commercially available Aziridine-2-carboxylates. Reduction of ester to aziridine-2-carboxaldehyde and the subsequent reaction with Ph3PCH2CO2R yielded cis-3-phenylethylaziridin-yl-acrylates in selective manner. Stereoselective dihydroxylation of 3-aziridin-2-yl-acrylates and regioselective ring opening reaction of aziridine ring afforded to the pyrrolidine-2-one with all right configuration.



1,4-Dideoxy-1,4-iminoribitol

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장소: 대구엑스코
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Efficient Synthesis of 3,4–Dihydroquinoxalin-2-amines EDTA-Catalyzed Three-Component Coupling in Aqueous Medium

KOLLA SRINIVASA RAO, 이용록

영남대 화학공학부

We describes a simple and efficient one-pot synthetic approach for the preparation of biologically interesting 3,4-dihydroquinoxalin-2-amine derivatives using EDTA-catalyzed three component reactions of o-phenylenediamines, carbonyl compounds, and isocyanides in an aqueous medium. This method is of great value because of its environmentally benign character, high yield, and easy handling.

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Syntheses and Properties of PCPP Derivatives Containing Benzothiadiazole for OPVs

심주영, *진영읍, 송수희, **이광희, 서홍석

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

The D-A type of alternating copolymers of PCPP-DTBT and PBEHPCPP-DTBT were synthesized by Suzuki coupling polymerization and characterized. The stable CPP unit was combined DTBT unit to generate the low energy level of the HOMO of the copolymer, which could be important for the generation of the high open circuit voltages (VOC) of the PSCs.Both of conjugated polymers showed significant absorbance up to around 700 nm region. The HOMO-LUMO energy bandgaps of these materials show 2.00 eV for PCPP-DTBT and 1.80 eV for PBEHPCPP-DTBT. Bulk heterojunction solar cells based on blends of the polymers with [6,6]phenyl-C71-butyric acid methyl ester (PC71BM) gave power conversion efficiencies of 1.00% for PCPP-DTBT and 1.12% for PBEHPCPP-DTBT under AM 1.5, 100 mW/cm2.

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Functionalized Liposome Microarrays for the Selective and Sensitive Sensing of Phosphate Derivatives

김경미, 안교한

포항공과대 화학과

Development of an efficient detection method for phosphate containing molecules has drawn significant interest because they are involved in various key biological processes such as metabolism, ATP hydrolysis, and DNA polymerization. Several notable fluorescent sensing systems have been developed recently. However, most known systems are small molecule based probes and thus operate in the homogenous state, whereas heterogeneous sensing systems remain to be explored, even though they have an obvious potential to be applied to chip-based assays. In our efforts to develop efficient molecular sensing systems, particularly turn-on fluorescence sensing systems for anions and metal cations,[1]we have investigated microarray chip systems based on poly(diacetylene) liposomes for the detection of phosphate-containing molecules. Thus, we have prepared the liposome based homogeneous sensing system for phosphate-containing analytes in aqueous media. From the stimuli-responsive liposomes, we have constructed a microarray chip assay system for the first time. A proper combination of the liposome components, analyte recognition ligands, and an anchoring component have been found to be important to obtain the microarray chip that selectively detects biologically important phosphate dervatives over other competing anions. We wish to present the chip-based assay that shows advantages over the solution-based ones in terms of high specificity and sensitivity.

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Syntheses and Characterizations of Low Bandgap Polymers Included Benzimidazole and Indenoindene for Solar Cells

심주영, 송수희, *진영읍, **이광희, 서홍석

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

The PININEDTMBI was used as the electron donor for the PSCs (ITO / PEDOT:PSS / polymer:PC71BM(1:4) /TiOx / Al). The unique structure of PININE, incorporating the vinylene unit with bicyclic [2.2.0] system, can overcome the basic degradation problem of the common type of vinylene units in PPV series. The solar cells made from conjugated PININEs with benzimidazole and thiophene units, which are new conjugated polymers for the application in polymer solar cells (PSCs), exhibit high PCEs even in basic PSC device structure. The best solar cell performance obtained has a layered structure of ITO / PEDOT:PSS / PININEDTMBI:PC71BM(1:4) / Al. Under white light illumination (AM 1.5 G, 100 mW/cm2), the obtained Jsc is 2.38 mA/cm2, Voc is 0.82 V, FF is 38%, and PCE is 0.76%. Study to improve the solar cell architecture and PCE is underway.

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발표분야: 유기화학

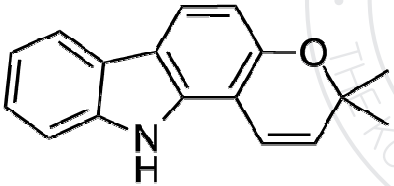
발표종류: 포스터, 발표일시: 목 10:30~12:30

Efficient Synthesis of Pyranocarbazole Derivatives by EDDA-Catalyzed Reaction

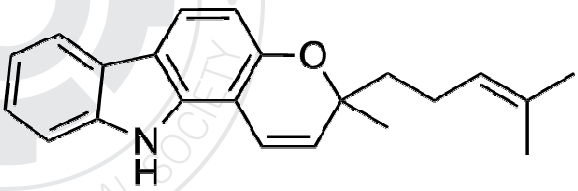
PANDIT RAMESHWAR PRA, 이용록

영남대 화학공학부

An efficient synthesis of pyranocarbazole derivatives was achieved by EDDA-Catalyzed reactions. These reactions provided a rapid entry to norgirinimbine and demethylmahanimbine.



Norgirinimbine



Demethylmahanimbine

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Enhanced Performance of Bulk Heterojunction Solar Cells Using New Conjugated Oligomers, DTBT Groups and Carbazole Unit

송수희, 손인영, 심주영, *이광희, 서홍석

*부산대 화학과 *광주과학기술원 신소재공학과*

The performance of organic photovoltaic (OPV) bulk-heterojunction blends comprising a liquid-crystalline fluorene derivative and a small-molecular fullerene is found to increase asymptotically with the degree of polymerization of the former. Interest in fluorene-based organic semiconductors has surged thanks to their ability to display high levels of (polarized) photoand electroluminescence as well as useful electronic chargetransport properties. More recently, a promising photovoltaic performance has been achieved through incorporation of such compounds in bulk-heterojunction blends. Both, oligo- and polyfluorene derivatives have been studied extensively and predominantly the latter have been found to display superior characteristics, such as significantly improved optical, electrochemical properties as well as for instance, the ability to form oriented fibers.Generally, one would expect that with increasing chain length most properties become less affected by small variations in the degree of polymerization, as indeed observed for the field-effect mobility, photoluminescence, as well as transition temperatures of various polyfluorenes.

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5-(6-Hydroxy-2-naphthyl)-1,2,3-benzenetriol : A Potent, New Tyrosinase Inhibitor

송수희, 손인영, 심주영, 서홍석

부산대 화학과

Tyrosinase inhibitors have become increasingly important in medication, cosmetic industry and food industry due to decreasing the excessive accumulation of pigmentation resulting from the enzyme action. Although a number of tyrosinase inhibitors are reported from both natural and synthetic sources, only a few of them are used as skin-whitening agents, primarily due to various safety concerns. For example, linoleic acid, hinokitiol, kojic acid, all naturally occurring hydroquinones, and catechols inhibit enzyme activity but also exhibit harmful side effects. Thus, melanin synthesis inhibitors may help treating localized hyper-pigmentation in humans. Epidermal and dermal hyper-pigmentation can be dependent either on an increased number of melanocytes or on melanogenic enzyme activity.Recently, our laboratory studied naphthalene-type resveratrol analogs, 6-(3-hydroxyphenyl)-2-naphthol and 4-(6-hydroxy-2-naphtayl)-1,3-bezendiol inhibited tyrosinase activity and reduced melanin in B16 cells, which indicated that these compounds could be depigmentation reagents. Furthermore, some hydroxystilbene compounds, including oxyresveratrol and resveratrol, can also inhibit tyrosinase activity.

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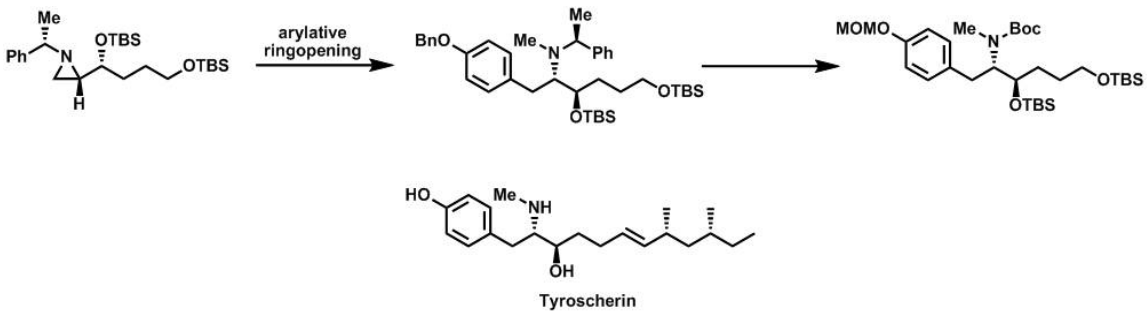
Formal Synthesis of Tyroscherin

윤두하, 하현준, *이원구

*한국외국어대 화학과 *서강대 화학과*

Recently we developed a method for the generation and the subsequent ring opening of the stable N-methylaziridium ion from 2-substituted [(1S)-phenylethyl]aziridine with various nucleophiles to yield cyclic and acyclic N-methylamines in enantiomerically pure forms. Application of this method allowed us for the formal synthesis of natural product tyroscherin isolated from the mycelium of Pseudallescheria sp. as a potent and selective inhibitor of IGF-1-dependent growth of MCF-7 human breast cancer cell. The key step of this synthesis involves methylation and the following arylative ring opening of [(1S)-phenylethyl]aziridine bearing a bis-1,4-t-butyldimethylsilyloxybutyl substituent with 4-benzyloxyphenylmagnesium bromide to yield provided the ring opened product. A formal synthesis of this natural product was succeeded by changing phenylethyl and benzyl group at the hydrogen and the phenyl ring to Boc and Mom, respectively.



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New Phosphorescent Iridium Complexes Comprising Imidazole Carboxylates as Ancillary Ligands

박혜정, 김경목, 윤웅찬

부산대 화학과

Recently phosphorescent iridium complexes attract more attention as emitting-materials for OLEDs because their highly efficient phosphorescence which originates from strong spin-orbit coupling leads to high internal quantum efficiencies in devices. In particular, FIrpic and its derivatives have attracted much attention because systematic fine control of the emission color can be possible by introduction of substituents or extension of π-conjugation on the main and (or) ancillary ligands. Based on the earlier observations, we deigned new iridium complexes which contain 2-(2,4-difluorophenyl)-4-methylpyridine and 2-(2,4-difluoro-3-trifluoromethylphenyl)-4-methylpyridine as main ligands, and the new imidazole carboxylates as ancillary ligands. The main ligands were prepared by utilizing a Suzuki coupling reaction and the new ancillary ligands were prepared following a modified method of the reported. The biscyclometalated Ir complex of main ligand was prepared by a conventional two-step reaction via μ-chloro-bridged dimer. Utilizing the synthesized two biscyclometalated Ir complexes and the new three ancillary ligands six blue-emitting heteroleptic Iridium (III) complexes were synthesized. Their structures were fully characterized by 1H- and 13C-NMR, high resolution mass spectroscopy and single crystal x-ray diffraction. Their UV-vis absorption and emission spectroscopy and electrochemical properties were investigated, and their quantum yields were measured. The synthesized iridium complexes with imidazole carboxylates as ancillary ligands exhibit strong phosphorescence (Φ= 0.03~0.5) with emission maxima in the region of reasonably deep blue 457~477 nm and show potential as blue phosphorescent dopants for OLEDs.

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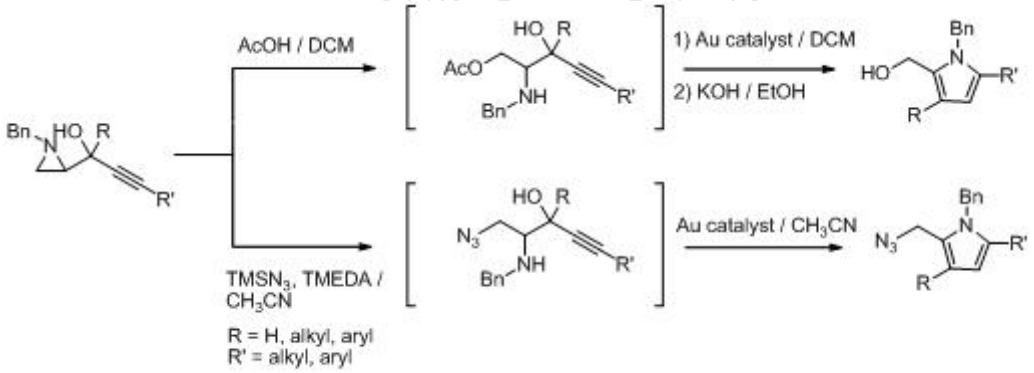
발표종류: 포스터, 발표일시: 목 10:30~12:30

An Efficient Synthesis of Substituted Pyrroles by Metal Catalized Reactions

김준희, 이백경, 이상빈, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

Pyrroles and substituted pyrroles can be found in various natural products and the importance of pyrrole derivatives is also found in pharmacologically and biologically active substances. we were interested in the new strategy for the efficient preparation of 1,2,- and 1,2,3-substituted-5-hydroxymethyl pyrroles from the sequential reactions including a ring-opening of 1-(aziridin-2-yl)propargylic alcohols by various nucleophiles followed by subsequent intramolecular cyclization of the aziridine nitrogen by metal catalyzed cyclization.



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Efficient Synthesis of Tetrahydroquinolinones by Brönsted Acid Catalyzed Formal [3 + 3] Cycloaddition

TO QUANG HUY, 이용록

영남대 화학공학부

A simple and efficient method for the synthesis of tetrahydroquinolinones was achieved by the reaction of various vinylogous amides with several α,β-unsaturated aldehydes. The key strategy was Brönsted acid catalyzed formal [3+3] cycloaddition.

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Characterization of Novel conjugated polymers based polyfluorene derivatives and C60as OPVs

박세정, *진영읍, 심주영, 서홍석, **이광희

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

New polyfluorene (PF)-based conjugated polymers, PC60BEHF, PC60BEHF-co-PDEHF containing chloro, azido, piperidine, and fullerene (C60) groups as pendants, were synthesized. The bulk heterojunction devices were fabricated with a typical device structure of ITO/PEDOT:PSS/composite film/Al.The band gap of polyfluorene is higher than MEH-PPV, and also acts as the barrier for the charge transfer between MEH-PPV to C60. As a result, the performance of the device using PC60BEHF-co-PDEHF, which has more amount of polyfluorene, showed the lower Jsc, Voc and FF as compared to those of the device using PC60BEHF. The photoinduced charge transfer from polyfluorene to covalently or ionically bound C60 occurred under photoexcitation and offers the possibility of the photovoltaic application of these materials. we can conclude that alkylated polyfluorene derivatives with C60 have a defect in electron transfer to electrode and too high bandgap for solar cells.

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Asymmetric Oganocatalysis Using Anodic Oxidation

xuanhuongho, 모선일, 장혜영

아주대 에너지시스템학부

Based on singly occupied molecular orbital (SOMO) concept, the enamine can be oxidized to render 3π-electron SOMO-activated species that can readily participate in a range of unique asymmetric bond construction. To perform SOMO catalysis, stoichiometric amounts of transition metal oxidants or inorganic oxidants have been used so far. With an aim to develop green catalytic reactions, electro-oxidation was employed for the enamine oxidation in asymmetric bond forming reactions. Through the anodic oxidation, large amounts of toxic chemicals can be avoided, leading to green chemistry. In this research, we studied the enatioselective α-alkylation and α-oxyamination of aldehydes via anodic oxidation. The catalytically competent intermediates and their electrochemical properties were also verified via cyclic voltammetry (CV).

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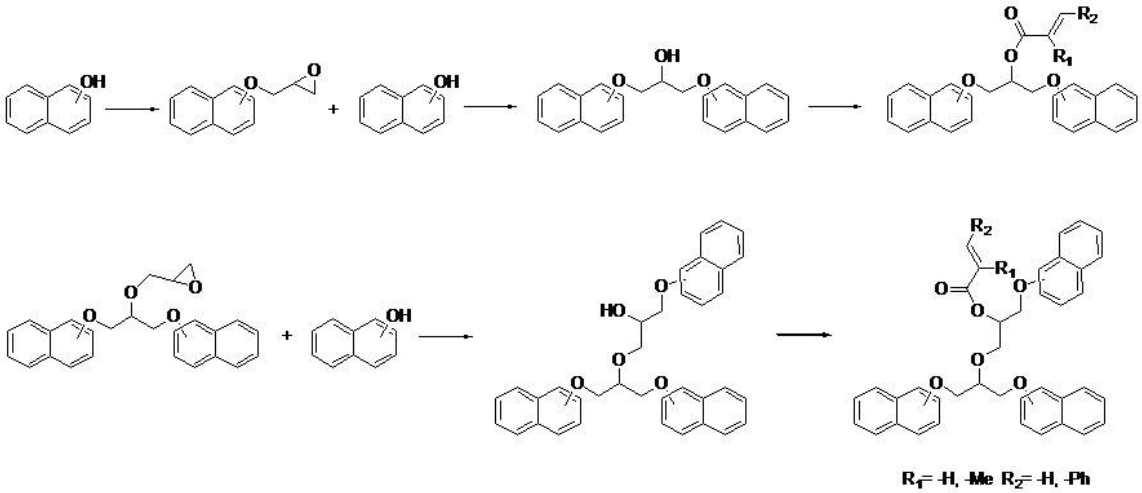
Functionalization of Aromatic Glycidyl Ether :Plausible materials for better LCD Back Light Unit

배정은, *이학준

*한양대 바이오나노학과 *한양대 응용화학과*

High Refractive acrylate monomers are used as material of 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. On the basis of this glycidyl ether, we added various acrylate, naphthoxy group, so we synthesized the high refractive acrylate monomers.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Characterizations of Novel Conjugated Polymer included CPDT for Solar Cells

박세정, *진영읍, 심주영, **이광희, 서홍석

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

These days, Many conjugated polymers for solar cells were synthesized. P3HT and PCPDTBT were successful OPVs. New type for OPVs is D-A polymers which have two absorption band in UV-vis absorption spectra. Recently, derivatives of PCPDTBT were synthesized and reported high photovoltaic properties. Herine, we designed and synthesized new acceptor material for D-A polymers. Novel conjugated polymer PCPDTMBI based on CPDT(cyclopentadithiophene) was synthesized by Stile coupling. The number molecular weight (Mn) of PCPDTMBI was 8.5 kg/mol, and the polydispersity index (PDI) was 2.1. UV-vis spectra of PCPDTMBI showed two band. Two λmax were 430 nm and 730 nm. Eopt was about 1.30 eV. The Phtpvoltaic property was Jsc(15mA/cm2),Voc(0.44V),FF(0.33) and Power conversion effciciency(PCE) is about 0.1%.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Asymmetric Formal Synthesis of Bromopyrrole Alkaloid Natural Products by Tandem Cross Metathesis/Intramolecular Aza-Conjugate Addition

권수현, 조창우

경북대 화학과

Pyrrolopiperazinones are one of key skeletons founded in bromopyrrole alkaloids which are a class of marine natural products with a variety of interesting biological activities. Examples of pyrrolopiperazinone alkaloids include hanishin, longamide B, longamide B methyl ester, cyclooroidin, and the agesamides. Although these pyrrolopiperazinone alkaloids have interesting biological activities and chemical skeletons and thus are potentially useful for the development of pharmaceuticals, asymmetric syntheses of the pyrrolopiperazinone alkaloids have been sparsely reported. Herein, we report a short and concise asymmetric formal synthesis of the known and overlapped key intermediate of pyrrolopiperazinone alkaloid natural products using tandem olefin cross metathesis/intramolecular aza-conjugate addition reaction as a key reaction.

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Organocatalytic Enantioselective Conjugate Addition Reactions of Pyrroles to α,β-Unsaturated Aldehydes

윤석호, 조창우

경북대 화학과

Synthesis of *N*-heteroaromatic compounds, especially optically pure ones, via catalytic routes has been a subject of active research. Recently, intensive efforts have been devoted to the development of organocatalytic asymmetric conjugate addition reactions. In organocatalytic asymmetric conjugate reactions, the use of *N*-centered heteroaromatic nucleophiles remains relatively unexplored in contrast to the widely studied *C*-centered nucleophiles. Herein, we report the first use of pyrroles as the *N*-centered heteroaromatic nucleophiles in the organocatalytic enantioselective conjugate reactions of α,β-unsaturated aldehydes.

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One-Pot Synthesis of Chiral Pyrrolizines by Organocatalytic Asymmetric Cascade Reactions

이효준, 조창우

경북대 화학과

Nitrogen-containing heterocycles and their derivatives have broad applications in organic, biological, and materials chemistry and, accordingly, synthesis of N-heteroaromatic compounds, especially optically pure ones, via catalytic routes has been a subject of active research. Recently, intensive efforts have been devoted to the development of organocatalytic asymmetric cascade reactions, because they provided powerful tools for the rapid and efficient construction of complex structures from simple precursors. Herein, we report the development of new organocatalytic asymmetric cascade reactions that afford highly functionalized chiral pyrrolizines which having potent cytostatic effects and thus are potentially useful for the development of antitumor and antiviral agents.

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Enantioselective Synthesis of Chiral Pyrrolidines by Organocatalytic Intramolecular Allylic Substitutions

허인정, 조창우

경북대 화학과

Various organocatalytic allylic substitutions, which proceed via a S_N2'-S_N2' tandem mechanism, have carried out with Morita-Baylis-Hillman (MBH) acetates using different types of nucleophiles. However, to the best of our knowledge, there are no report on the intramolecular version of the organocatalytic allylic substitutions of MBH acetates, although these reactions afford versatile heterocyclic intermediates for pharmaceutical and natural product synthesis. Herein, we report the first intramolecular organocatalytic asymmetric allylic substitutions of MBH acetates containing a protected amine moiety (nucleophile) to afford various chiral 2-(α-methylene)-pyrrolidine derivatives which are important moieties of a large number of pharmaceuticals and biologically active natural products.

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Enantioselective Formal Synthesis of Bromopyrrole Alkaloid Natural Products by Organocatalytic Conjugate Addition Reactions

이수정, 조창우

경북대 화학과

Bromopyrrole alkaloid natural products are a class of marine natural products with a variety of interesting biological activities. Although these bromopyrrole alkaloids bearing pyrrolopiperazinone skeletons have interesting biological activities and chemical skeletons and thus are potentially useful for the development of pharmaceuticals, asymmetric syntheses of the pyrrolopiperazinone alkaloids have been sparsely reported. Therefore, the development of a new route for the efficient synthesis of pyrrolopiperazinone alkaloids is highly desirable. Herein, we report a concise enantioselective formal synthesis of the known and overlapped key intermediate of pyrrolopiperazinone alkaloid natural products using organocatalytic asymmetric conjugate addition reactions as a key reaction.

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Novel D-A Oligomers Based on Carbazole and Benzimidazole Derivatives for Solar Cell

한효정, 송수희, 심주영, 서홍석, *이광희

*부산대 화학과 *광주과학기술원 신소재공학과*

Recently, a promising photovoltaic performance has been achieved through incorporation of such compounds in bulk-heterojunction blends. BHJ films have been dominated by polymeric donor materials, as they typically have better characteristics than their small-molecule counterparts. Small molecules do not suffer from batch to batch variations, broad molecular-weight distributions, which can be significant problems for polymer. So, we synthesized a non-polymeric, Carbazole and Benzimidazole Derivatives that can be solution processed with a fullerene acceptor to produce good quality films is reported.

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A photochromic phenoxyquinone cyanide chemosensor system

허은주, 박인성, *김종만

*한양대 화학공학과 *한양대 응용화공생명공학부*

시안화 이온은 강한 독성을 지니며 인체에 매우 해로운 것으로 알려져 있다. 시안화 이온이 체내에 흡수되면 세포호흡을 담당하는 효소인 시토크롬옥시다아제의 철 이온과 반응하여 세포호흡을 중단시켜 세포괴사를 일으키게 된다. 본 연구에서는 친핵성을 가지는 시안화 이온의 성질을 이용하여 이를 선택적으로 검출할 수 있는 센서를 설계하였다. 페녹시퀴논 유도체는 광변색화합물 중에 하나로써 형광패턴, 분자 스위치 등으로 응용이 가능하다. 이 물질에 특정 파장대의 빛을 조사하면 벤젠 그룹이 이동하면서 trans 형태에서 ana 형태로 변화하는 광화학적 재배열이 일어난다. ana 형태로 이성질화되면 페녹시 그룹이 연결된 C-O 결합의 탄소가 매우 친전자성을 띄게 된다. 이때 여러 종류의 음이온을 넣어주면 시안화 이온에서만 600nm-1000nm 파장대의 흡광도가 증가하고 이를 통해 시안화 이온을 선택적으로 검출할 수 있음을 확인할 수 있다. 이것은 중간체의 흡수 스펙트럼으로써 시간이 지나면 다시 감소하게 된다. 본 연구의 최종물질로 페녹시퀴논과 시안화 이온이 1:2 로 결합한 시안화 첨가물을 얻었다. 우리는 시안화 이온의 화학결합을 통해 시안화 이온에만 특이적으로 흡수파장을 가지는 화학센서를 개발하였다.

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Synthesis and Characterization of new PCPP -based conjugated polymers BT unit for Organic Light-emitting Diodes

신현민, 송수희, *진영읍, 심주영, **이광희, 서홍석

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

The new copolymers, PCPPBTs, were synthesized by the Suzuki coupling reaction from 4H-cyclopenta[def]phenanthrene (CPP) and BT. The donor-acceptor copolymers, PCPPBTs, were synthesized by the Suzuki coupling reaction. The experimental results suggest that the acceptor contents affect the electronic and optoelectronic properties including the optical band gap, LUMO level, and luminescence maximum. The intensities of the blue-emitting peaks were decreased, while those of the green-emitting peaks were increased. The emissive colors were green and the peaks by the PCPP segments were nearly quenched. The HOMO energy levels of the copolymers ranged from -5.89 to -5.96 eV, and the LUMO energy levels were about -3.33 to -3.50 eV. The polymer LEDs of PCPPBTs with the configuration of ITO/PEDOT/polymer/Ca:Al emitted light with maximum peaks at 508-528 nm. Among all the devices fabricated, the best device was the one with PCPPBT10, which showed the highest luminous efficiency of 1.25 cd/A and the highest brightness of 1170 cd/m2.

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Low-Bandgap Benzimidazole Derivatives for Organic Photovoltaic Cells

신현민, 송수희, *진영읍, 심주영, **이광희, 서홍석

*부산대 화학과 *부경대 공업화학과 **광주과학기술원 신소재공학과*

BHJ films has been dominated by polymeric donor materials, as they typically have better film-forming characteristics and film morphology than their small-molecule counterparts.A thin film of PCDTMBI, containing the dimethyl-2H-benzimidazole unit, shows two broad absorption bands with maxima at 400 and 636 nm and an absorption onset of 756 nm,corresponding to a band gap of 1.64 eV. The oxidation onset of PCDTMBI was estimated to be 0.67eV, which corresponds to a HOMO energy level of −5.47 eV. The LUMO energy level of the polymer was thus determined to be −3.82 eV. A device with a PCDTMBI:PC71BM blend had a VOC value of 0.65 V, a JSC value of 10.0 mA/cm−2, and a FF of 0.48, leading to an efficiency of 3.12%. The enhanced efficiency of PCDTMBI was caused by the higher IPCE value between 400 and 700 nm and high mobility (2.2 × 10−3 cm2 V−1/s−1).

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Synthesis and Characterization of HNB as a New Tyrosinase Inhibitor

송수희, 한효정, 심주영, 서홍석

부산대 화학과

Tyrosinase is a important enzyme for melanin biosynthesis and known to be sensitive to UV light in the presence of oxygen. Therefore, finding effective tyrosinase inhibitors can be useful in the treatment of melanin-related disorders.So, We synthesized HNB(4-(6-Hydroxy-2-naphthyl)-1,3-bezendiol). In a kinetics study, HNB was identified as a competitive inhibitor of the mushroom tyrosinase with the same Vmax value. Therefore, HNB might indicate the enzyme inhibitory activity by binding at the same site as the copper active site of mushroom tyrosinase. Newly synthesized HNB is a safe andeffective tyrosinase inhibitor that can be produced in large quantities. We propose HNB as a potent new tyrosinase inhibitor that could be considered for skin lightening purposes.

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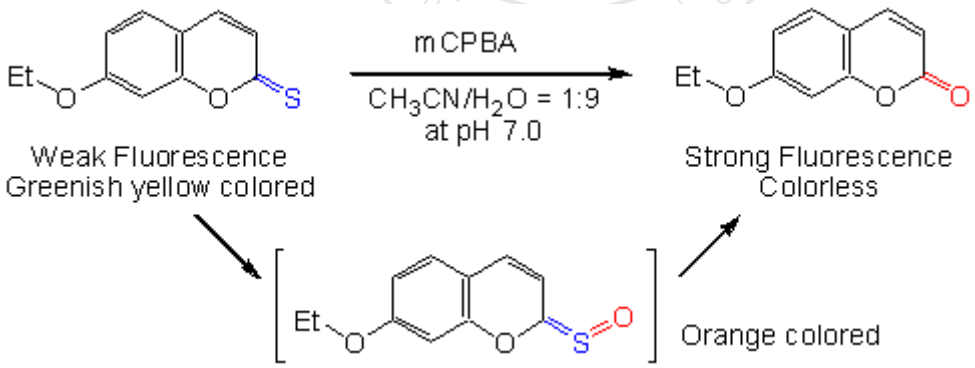
Dual signaling of m-chloroperbenzoic acid by desulfurization of thiocoumarin

차선영, 황지영, 최명길, 장석규

중앙대 화학과

m-Chloroperbenzoic acid (mCPBA) chemosignaling system based upon thiocoumarin was investigated. Signaling was due to the efficient desulfurization of thiocoumarin to coumarin by mCPBA. Thiocoumarin exhibited very efficient mCBPA signaling in the presence of common alkali and alkaline earth metal ions as well as anions with a detection limit of 6.8 μM in a 90% aqueous acetonitrile solution. Thiocoumarin also exhibited mCPBA-selective signaling in the presence of a large excess of widely used oxidant of hydrogen peroxide.



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Chromogenic Signaling of Water Content in Organic Solvents by Hydrazone–Acetate Complex

김윤환, 최명길, 박지은, 장석규

중앙대 화학과

New chromogenic probe system for the signaling of water content in representative water miscible organic solvents was investigated. Effect of water content in organic solvents on the complex formation of hydrazone dye with acetate ion was utilized for the signaling. The hydrazone–acetate system exhibited a pronounced chromogenic signaling behavior in response to the changes in water content in common water miscible organic solvents of acetonitrile, THF, and DMSO. Developed system also exhibited fluorescence changes but the signaling profile was not so informative as absorption behavior.

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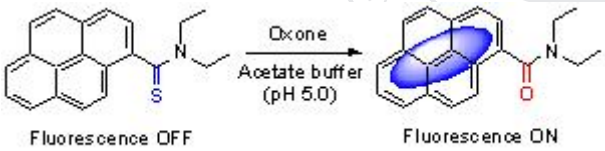
Fluorescent Signaling of Oxone by Desulfurization of Thioamide

어수영, 황지영, 최명길, 장석규

중앙대 화학과

The chemosignaling of the oxidant Oxone by selective desulfurization of a thioamide was investigated. Pyrene-thioamide was selectively converted to its amide analogue by reaction with Oxone, resulting in a pronounced fluorescent turn-on-type signaling. Selective signaling of Oxone in aqueous solution was possible in the presence of representative alkali and alkaline earth metal ions, as well as common anions. The thioamide also exhibited Oxone-selective signaling behavior over the widely used oxidant hydrogen peroxide.



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Synthesis of Whitening Agents Using Benzene Derivatives

최형, 한병희, 강성권

충남대 화학과

Tyrosinase is known to be a key enzyme in melanin biosynthesis, involved in determining the color of mammalian skin and hair. In the course of our work on the development of new whitening agents, a series of N-hydroxy-N‘-phenylthiourea and N-hydroxy-N’-phenylurea analogues were prepared and evaluated as a inhibitors of tyrosinase and melanin formation.

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Synthesis of novel blue photoluminescence compound based on the bis 2-(4-(diphenylphosphino)phenyl)benzo[d]oxazole

TRINH DAC HOANH

인제대 화학과

A novel compound, bis 2-(4-(diphenylphosphino)phenyl)benzo[d]oxazole (BPB), was synthesized and applied in organic light emitting diodes (OLED). Although OLEDs have a lot of advantages to compare with other display technologies such as thinner, brighter, low power consumption, etc., the lifetime, luminance efficiency and other OLED properties still should be improved, especially the lifetime of blue emitting materials. The structure of BPB was determined by 1H-NMR, 13C-NMR, FT-IR, UV-Vis, XPS and elemental analysis. BPB shows the blue emission under excitation by UV lamp of 365 nm and the photoluminescence maximum at 410 nm. The electroluminescence (EL) properties will be discussed. References[1] C.W. Tang, S.A. Van Slyke, Appl. Phys. Lett. 51, 913 (1987).[2] J.H. So, J.P. Heeschen. J.Org. Chem 62, 3552 (1997).[3] E.Orseilli, G.S.Kottas, A.E.Konradsson, P.Coppo, R.Frolich, L.D.Cola, A.V.Dijken, M.Buchel, H.Borner, Inorg.Chem. 46,11082 (2007).

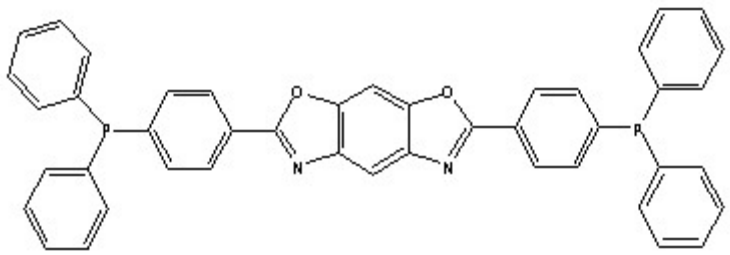

Fig 1. Chemical structure of BPB

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Synthesis of novel linear ARCA for produce D-amino acid

이선민, *이예정, **김관묵

*이화여대 화학 나노과학과 *이화여대 화학나노과학과 **이화여대 화학과*

Enantiomeric recognition of amino acids has been extensively studied because of their importance as biologically active molecules and as ligands for stereoselective catalysts. 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. In the past years, we developed several binol based receptors for amino alcohols and amino acids called as ARCA systems. On continuation of our work, we report here a novel ARCA receptor which has many advantages such as solubility in organic solvents and high enantioselectivity towards the chiral amino alcohols and amino acids, compared to the other developed receptors. These receptors enantioselectively binds an amino acid and converts L-amino acid to D-amino acid. Hence, D-amino acids can be produced in large scale under operationally convenient conditions without inert atmosphere, rigorously dried/degassed solvents, or difficult-to-maintain temperatures. Furthermore, they are used to enantioselectively recognize various 1,2-amino alcohols. The synthetic details of these receptors, the molecular recognition properties studied by 1H NMR and the production of D-amino acids will be presented.

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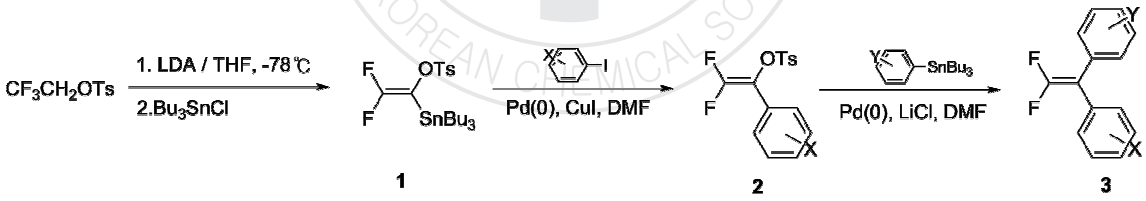
Direct Consecutive Coupling Reactions of 2,2-Difluoro-1-tributylstannylethenyl *p*-Toluenesulfonate with Aryl Iodides

한승연, 정인화

연세대 화학및의화학과

2,2-Difluoro-1-tributylstannylethenyl *p*-toluenesulfonate 1 was reacted with aryl iodides in the presence of 10mol% $Pd(PPh_3)_4$ and 10mol% CuI in DMF at 80℃ for 10~20 h to give the cross-coupled products 2 in 35~97% yields. Further coupling reactions of 2 with arylstannanes in the presence of 5mol% $Pd(PPh_3)_4$ and 3 equiv LiBr in DMF heat at 100℃ for 2~24h afforded the desired products 3 in 25~78% yield. The scope of these coupling reactions will be presented.



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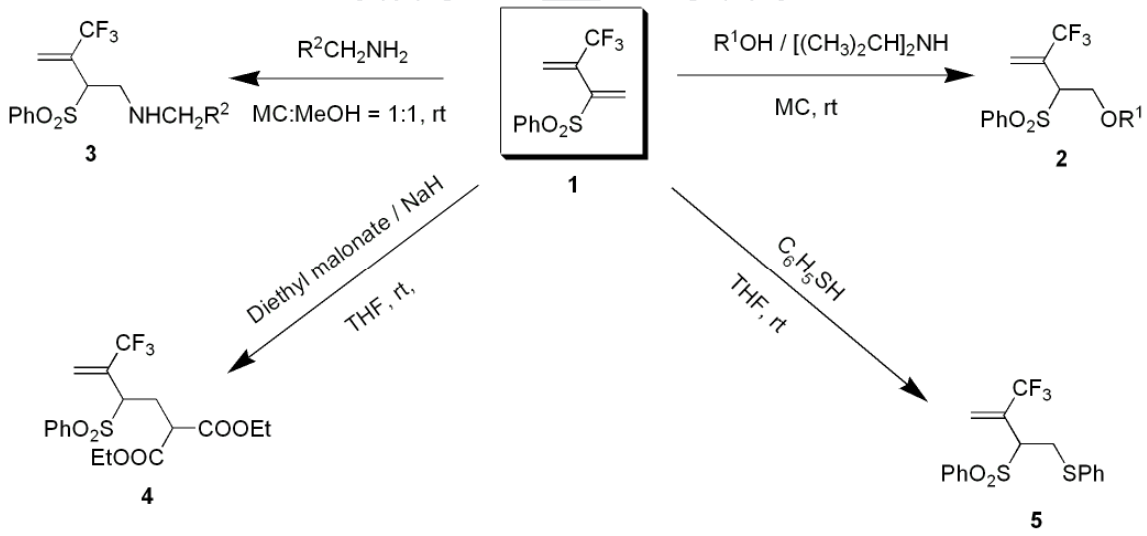
발표종류: 포스터, 발표일시: 목 10:30~12:30

Nucleophilic Reactions of 2-Trifluoromethyl-3-phenysulfonyl-1,3-butadiene

양은준, 정인화

연세대 화학및의화학과

Reaction of 2-trifluoromethyl-3-phenylsulfonyl-1,3-butandiene 1 with alcohols in the presence of diisopropylamine provided the alcohol addition products 2 in excellent yield. When this reaction was performed in the presence of primary amine, however, amine addition products 3 were obtained in good yields. The reaction of 1 with sodium malonate or thiophenol afforded the addition product 4 or 5 in good yield.



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Catalytic Approach to the Total Synthesis of Fluvastatin

김애진, 박언정, 박지혜, 김인수

울산대 화학과

Statins, 3-hydroxy-3-methylglutaryl-coenzyme A (HMG-CoA) reductase inhibitors, have become the most frequently prescribed agent for the treatment of hypercholesterolemia due to the compelling evidence of their effect on reducing the rates of cardiovascular events. In particular, Fluvastatin (Lescol) inhibits the enzyme that reduces 3-hydroxy-3-methylglutaric acid to mevalonic acid, thus blocking the biosynthesis of cholesterol and lowers low-density lipoprotein cholesterol levels by 20-30% at a daily dose of 20-40 mg. Because of their potent pharmacological effects and interesting structural features, statins have attracted considerable attention as powerful synthetic targets.In this paper, we wish to demonstrate a concise asymmetric synthesis of Fluvastatin via enantioselective iridium-catalyzed carbonyl allylation from the aldehyde oxidation level. The total synthesis of Fluvastatin was accomplished in 10 steps from readily available indole and the key steps in the route involve iridium-catalyzed arylation of sp2 C-H bond, iridium-catalyzed asymmetric allylation, ruthenium-catalyzed intermolecular olefination, and base-catalyzed intramolecular Michael addition.

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Synthesis of Fréchet-type Denderimers viaNew Double Click Chemistry

이재욱, 지원호, 한승철

동아대 화학과

The well-known click chemistry which is useful tool for synthesis of dendrimers, is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition proved to be an ideal reaction in very good to excellent yields. Staudinger/aza-Wittig reactions (new click reaction) between azide and aldehyde are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Taking advantage of these facts, herein we will use the first 1,3-dipolar cycloaddition reaction with azide-dendrons leading to the aldehyde-functionalized Fréchet monodendrons containing the 6-hexanal at a core, and then will use the second Staudinger/aza-Wittig reactions with azide-dendrons leading to the formation of Fréchet-type dendrimers.

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Convergent Synthesis of Unsymmetrical dendrimers via Double Click Reactions of the Fréchet-type Dendrons

이재욱, 박다정, 한승철

동아대 화학과

The well-known click chemistry which is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition, is useful tool for synthesis of dendrimers because it was proved as an ideal reaction to obtain very good to excellent yields. Staudinger/aza-Wittig reactions (new click reaction) between azide and aldehyde are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Taking advantage of these facts, herein we will use the first click reaction (Staudinger/aza-Wittig reaction) leading to the alkyne-functionalized Fréchet monodendrons containing the benzene at a core, and then will use the second click reaction (1,3-dipolar cycloaddition reaction) with azide-dendrons leading to the formation of unsymmetrical Fréchet-type dendrimers.

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Convergent Synthesis of Unsymmetric Fréchet-type Poly(arylether) Dendrimers Using Staudinger/aza-Wittig Reactions

이재욱, 송태규, 한승철

동아대 화학과

A convergent synthetic method for the synthesis of Fréchet 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 unsymmetric Fréchet-type poly(arylether) dendrimers via Staudinger/aza-Wittig reactions (new click reaction) between azido-focal dendrons and aldehyde-focal dendrons. The dendrimers were characterized by ^{1}H and ^{13}C NMR spectroscopy, IR spectroscopy, and mass spectra as well as GPC analysis.

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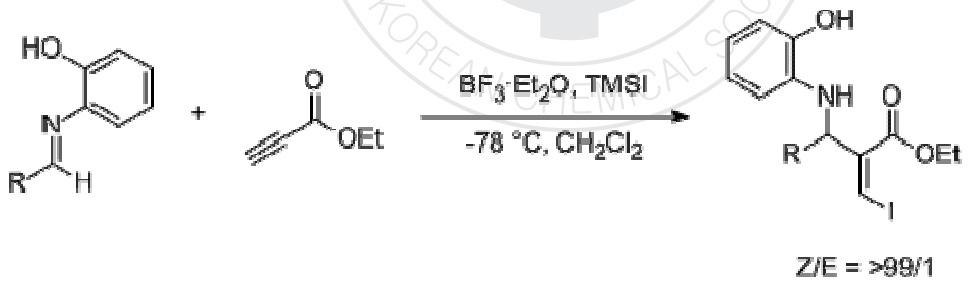
Highly Z-Stereoselective Synthesis of β-Iodo aza-Morita–Baylis–Hillman Esters with imines as Aldol Acceptors

이성일, *정재아, *박지호, *조성호, *조나연, 류도현

*성균관대 화학과 *경기과학고 화학과*

Boron trifluoride-TMSI has been found to promote the efficient and highly stereoselective synthesis of (Z)-β-iodo-α-(aminoalkyl) acrylates via one-pot three-component coupling reactions. This new system has made it possible to utilize various imines as the electrophiles, in order to react with an trimethylsilyl allenoate intermediate for the synthesis of β-iodo aza-Morita–Baylis–Hillman adducts with high yield and excellent Z-stereoselectivity (>99%).



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Synthesis and Photophysical, Electrochemical and Thermal Properties of a Series of Iridium(III) Complexes Containing Trimethylsilan Group

강현희, 오대환, 소기호, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Luminescent complexes containing third-row transitionmetals have attracted much attention owing to their varied applications, such as photonics and electronics. In particular, cyclometallated iridium(III) complexes are regarded as excellent phosphorescent materials and have been widely studied because of their ability to achieve maximum internal quantum efficiency, nearly 100%, as well as high external quantum efficiency in OLEDs.To achieve full color display, three primary colors, such as blue, green, and red, are necessary. However, Ir(III) complexes with both blue emission is very rare, compared to those of phosphorescent green and red. The following considerations should be needed for the development of blue phosphorescent Ir(III) complexes: (i) the adoption of a ligand with large triplet energy, since the emission energies of cyclometallated Ir(III) complexes are mainly determined by the triplet energy of the C∧N chelating ligand, and (ii) the inducement of a larger band gap by stabilizing the HOMO and destabilizing the LUMO level.In this research, we designed and synthesized new iridium complex. And the physical properties of new iridium complex will be discussed.

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Systematic Structure-Property Investigations Studies of Donor/Acceptor Tetrakis(arylethynyl)pyrene

이연옥, 김종승

고려대 화학과

Structural isomers of a tetrakis(arylethynyl)pyrene chromophore functionalized with dimethylaniline and trifluorophenyl units as respective donors and acceptors have been synthesized and their steady state spectroscopic parameters investigated. The effects of small structural variations on the electronic absorption and emission spectra have been explored in evaluation of their potential as optical materials components. These structural variations have predictable consequences and thus allow fine-tuning of the optoelectronic properties for specialized applications

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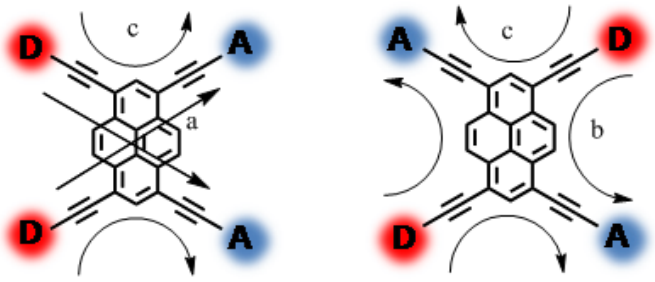

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Colorimetric Detection of chemical warfare agent by Azo derivative

김현정, 이재홍, 김종승

고려대 화학과

Synthesis of donor–acceptor azo derivative 1 and its chromogenic behavior for DCP in acetonitrile were investigated. Significant changes in UV–visible absorbance wavelength indicate the effectiveness of 1 as a DCP sensor. Upon DCP binding, 1, bearing a pyridyl group, exhibited a marked red-shifted absorption band ($\Delta\lambda$=60 nm). The solution of 1 could be fully regenerated by rinsing with 0.01 M NaOH, with which the quaternary pyridinium returnes to the pyridine form.

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A New Fluorescent Chemosensor for Mercury(Ⅱ) Ion Recognition

정혜정, **LIYINAN**, 현명호

부산대 화학과

A new fluorescent compound prepared from 4-chloro-7-nitrobenzofurazan (NBD) and bis(2-(ethylthio)ethyl)amine was investigated for its metal ion selective fluorescent chemosensing behavior. The new compound exhibits a notable fluorescence enhancement for Hg2+ in aqueous 50% acetonitrile with respect to the selective phosphorescent detection of various metal ions including Ag+, Ba2+, Ca2+, Cs+, Cu2+, Fe2+, K+, Li+, Mg2+, Na+, Zn2+ and Hg2+. The fluorescent titration for Hg2+ shows a blue shift compared with other ions.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

An Phosphorescent iridium (III) complex Based chemosensor for Anion Sensing

LIYINAN, 현명호

부산대 화학과

A new phosphorescent iridium (III) complex was prepared and its aion selective phosphorescent chemosensing behavior was investigated. The new iridium (III) complex examined for its anion binding ability toward various aions including F-, Cl-, Br-, I-, HSO4-, H2PO4-, and OAc- by the phosphorescent spectroscopy in acetonitrile solution. The addition of an anion to the iridium (III) complex resulted in a change in phosphorescent intensity at the excitation of 372 nm. Analysis of the job`s plot spectral suggested that the ligand formed a 1:1 complex with each of the anions, showing strong affinity for dihydrophosphate in acetonitrile.

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(S)-Benzyl-isothiouronium chloride as an effective organocatalyst for the direct reductive amination of aldehydes

N.P.B.Quynh, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부 광바이오사업단*

The reductive amination is one of the most powerful methods for the synthesis of amines. The versatile coupling reaction enables a rapid and general access to C-N bonds, a key structure feature in natural products and pharmaceuticals. Particularly, the 'one-pot' fashion in which carbonyl component is treated directly with the amine and the reducing reagent has been developed by a number of methods such as using Bronsted or Lewis acids. However, application of the protocols to sensitive, acid-labile or polyfunctional substrates is limited. Herein, we wish to report the direct reductive amination of aldehyde by using (S)-benzyl-isothiouronium chloride as a catalyst for the activation of imine through the hydrogen bonding. A mild and operationally simple fragment coupling has been accomplished with a wide range of aldehydes as well as amines in good to excellent yield. In addition, the catalyst (S)-benzyl-isothiouronium chloride can be easily recovered and reused without significant change. Therefore, it can be recognized as an effective catalyst for the direct reductive amination of aldehydes.

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Asymmetric alkylation reactions using benzene-based dipodal 2-phenyl amino-2-oxazolines as chiral auxiliaries

정송이, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부 광바이오사업단*

Chiral auxiliary-derived asymmetric alkylations have been extensively studied and are now important and general methods for asymmetric carbon-carbon bond formation. In particular, metal enolates of N-acyl oxazolidinones, developed by Evans, are highly effective in controlling facial selectivity for the preparation of homochiral α-substituted carboxylic acid and their derivatives. However, this auxiliary undergoes endo-cylic cleavage rather than the required exocyclic cleavage in the alkaline hydrolysis. To suppress this trouble, we reported the novel chiral auxiliary based on 2-phenylamino-2-oxazoline which exhibited excellent level of stereocontrol, greater stability and recyclability. Since the success in the mono case, in this study, we wish to investigate the asymmetric alkylation reactions in dipodal case by develop the benzene-based dipodal 2-phenyl amino-2-oxazoline chiral auxiliaries. As expected, the asymmetric benzylation and allylation reactions proceeded well with high stereoselectivity (d.e >99%). However, in case of asymmetric methylation, lower stereocontrol (d.e 70%) was obtained as compared with the mono case. Several cleavage conditions were also examined for the parallel synthesis of several chiral acids, esters and alcohols.

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High-Efficient Blue Phosphorescence Host Material by Solution-Process

오대환, 강현희, 소기호, *이태우, **권순기, 김윤희

*경상대 화학과 *포항공과대 신소재공학과 **경상대 나노신소재공학부*

OLEDs, getting the spotlight as a next generation display spends less eletric power compared with other displays, and it is the most suitable display for realizing flexible display, if it has high efficiency, quick response speed and wide viewing angle. In this research, we adopted tetraphenylsilane moiety for wide energy band gap(Eg), thermal-chemical stability, high efficiency and stability of a device. Diphenyl-bis(3-(pyridine-2-yl)phenyl)silane (BPOTPS), was synthesized for blue phosphorescent organic light emitting diodes (OLEDs) and BPOTPS was fabricated by solution-process.

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Novel fused-ring mesoionic systems based on thieno[1,2,4]triazolo[4,3-c]pyrimidines

송양헌, 이한미

목원대 화학과

A variety of monocyclic mesoionic compounds are known, but derivatives containing fused mesoionic rings are less common, especially those with the second ring heteroaromatic. We have attempted to synthesize some of new fused-ring mesoionic systems based on thieno[1,2,4]triazolo[4,3-c]pyrimidines. The reaction of thieno[1,2,4]triazolo[4,3-c]pyrimidine-3(2H)-thione with phenylbromoacetic acid under basic condition readily gave the corresponding carboxybenzylthio derivatives. These were smoothly converted into the new corresponding mesoionic systems by treatment with DCC or acetic anhydride in the presence of Et3N.

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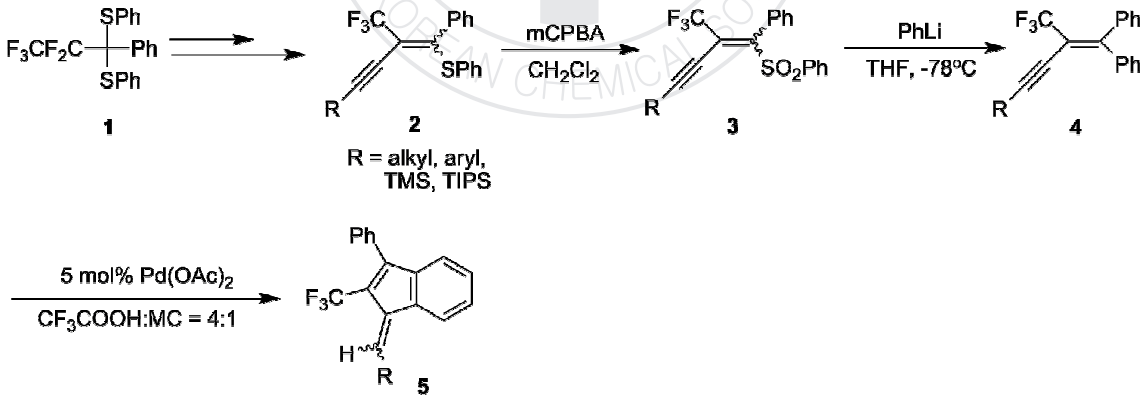
Cyclization reaction of 1-phenyl substituted 2-trifluoromethyl-1,3-enynes

홍윤영, 정인화

연세대 화학및의화학과

2-Trifluoromethylated enynyl sulfides 2 were prepared in 1~2 steps from pentafluoroethyl phenyl dithioketal 1. After oxidation of 2, the resulting compounds 3 were reacted with PhLi at -78℃ to give 1,1-diphenylated 1,3-enynes 4 in good yields. Cyclization reaction of 4 in the presence of 5 mol% $Pd(OAc)_2$ in a mixture of CF_3COOH and CH_2Cl_2(4:1) at room temperature for 1 h provided the corresponding indene derivatives 5 as an *E* & *Z* isomeric mixture.



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Kinetic Study with *t*-Butyl Chlorothioformate under Solvolytic Conditions

이예린, 성미혜, 원호식, *경진범

*한양대 응용화학과 *한양대 과학기술대학 응용화학과*

The specific rates of solvolysis of *t*-butyl chlorothioformate(*t*-BuSCOCl) are analyzed in 20 solvents of widely varying nucleophilicity and ionizing power at 25.0 °C using the extended Grunwald-Winstein equation [log(*k*/*k*o)= $lN + mY + c$]. The sensitivities (l and m-values) to changes in the N_T solvent nucleophilicity scale and the Y_{Cl} solvent ionizing power scale are similar to those for solvolysis of *i*-propyl chlorothioformate (*i*-PrSCOCl), consistent with the ionization pathway being rate-determining. For four representative solvents, studies were made at several temperatures and activation parameters determined. These observations are also compared with those previously reported for the corresponding primary and secondary alkyl chlorothioformates.

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Correlation of the Specific Rates of Solvolysis of 1- and 2-Naphthyl Chloroformates Using the Extended Grunwald-Winstein Equation

문두환, 최송희, 이용우, 경진범

한양대 응용화학과

The specific rates of solvolysis of 1- and 2-naphthyl chloroformates have been measured at 2.0°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 the N_T solvent nucleophilicity scale and the Y_{Cl} solvent ionizing power scale, and the solvent isotope effect, k_{MeOH}/k_{MeOD} ratio is very similar to those for solvolyses of *p*-nitrobenzyl chloroformate, consistent with the addition step of an addition-elimination pathway being rate-determining which is accompanied by general-base catalysis. For four representative solvents, studies were made at several temperatures and activation parameters determined. The results are also compared with those reported earlier for alkyl haloformate esters and mechanistic conclusions are drawn.

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Synthesis and Characterization of New Blue Light Emitting Material with Limb Structure

배만훈

경상대 화학과

Organic Light Emitting Diodes (OLEDs) has several characteristics: consuming a lower amount of electronic power; high quality of efficiency; a rapid response speed to the results; and a broad angle of view of things. That is why OLED is one of the most popular displays in these days. Blue color emitting light materials have a diversity of problems to be improved compared with red color and green color materials. That is because it is hard to materialize high color purity, which must have high efficiency.In this paper, we report the synthesis and characterization of a novel, deep-blue-emitting material, 2,3-bis(9,9-diethyl-9H-fluoren-2-yl)-9,10-di(naphthalen-2-yl)anthracene. In this material, two fluorene groups and two naphthalene groups are end-capped at the 2-, 3-, 9- and 10-positions of the central anthracene core to increase structural bulk and non-planarity through the tendency of the phenyl rings to twist. The non-planarity of this molecular structure effectively diminishes its degree of intermolecular p–p stacking.

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Phosphorescent OLEDs Using Iridium(III) Complexs with Phenylpyridine Ligands Contaning Trimethylsilyl Group

소기호, 배만훈, 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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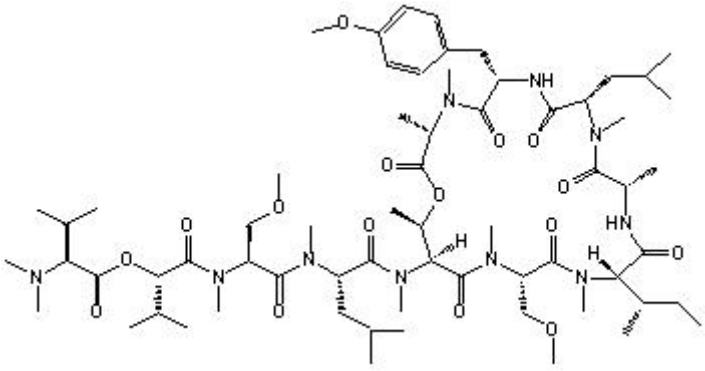
고체상 합성을 이용한 Coibamide A의 합성에 관한 연구

전혜영, 박재관

세종대 화학과

Cyclic depsipeptide 계열인 Coibamaide A 는 해양의 cyanobacterium 인 Leptolyngbya ap.에서 분리된 이 물질은 암세포에 대한 IC50 가 2.8~7.6 nM 인 매우 강력한 항암활성을 갖는다. 현재 cell cycle 에서 G1 phase 를 증가시키는 물질로만 알려져만 있으며 아직 합성이 보고된 바 없기 때문에, 합성이 이루어지면 구조에 대한 stereochemistry 를 확인 할 수 있으며 아직 밝혀지지 않은 anticancer mechanism 에 대한 연구도 가능하다. Coibamide A 는 7 개의 N-methyl 아미노산을 포함하고 있어 용액상에서 반응 시 각각의 coupling 반응에 대한 효율이 떨어지고, cis-trans isomer 의 존재로 중간단계마다 분리와 정제과정에서 문제가 발생할 수 있기 때문에 Trityl resin 을 지지체로 사용하여 Fmoc chemistry 에 기초한 고체상합성법을 이용하여 합성하였다. 합성과정은 Tyr 유도체를 이용하여 resin 에 연결한 후, 나머지 아미노산을 연결 합성하여 cyclization 을 수행하였다. 그리고 나머지 N-methyl 아미노산을 coupling 하고 resin 을 제거한 후, 용액상에서 Tyr methylation 을 통하여 최종 화합물을 얻고자 하였다.



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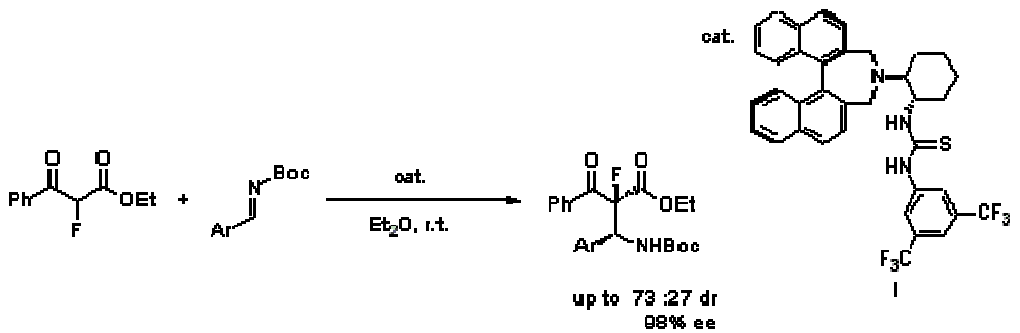
Organocatalytic highly enantio- and diastereoselective Mannich reaction of α-fluoro-β-ketoester with N-Boc-aldimines

윤성제, 김대영

순천향대 화학과

The chemistry of chiral organofluorine compounds is a rapidly developing area of research because of their importance in biochemical and medicinal application. The Mannich reaction is a fundamental C-C bond-forming reaction in synthetic organic chemistry. Catalytic enantioselective Mannich reactions provide one of the most versatile and attractive approaches for the generation of optically active chiral β-amino acid derivatives The catalytic enantioselective Mannich reaction promoted by chiral bifunctional organocatalysts is described. The treatment of α-fluoro-β-ketoester with N-Boc-aldimines under mild reaction conditions afforded the corresponding β-amino β-ketoesters with excellent diastereoselectivities and enantioselectivities (up to 98% ee).



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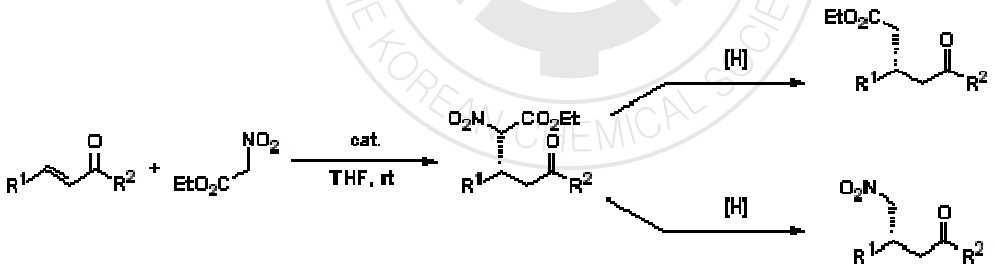
Enantioselective conjugate addition of nitroacetate to α,β-unsaturated ketones catalyzed by chiral bifunctional organocatalyst

문형욱, 김대영

순천향대 화학과

The catalytic enantioselective conjugate addition reaction of nitroacetate to α,β-unsaturated ketones promoted by chiral bifunctional organocatalysts is described. Treatment of nitroacetate to α,β-unsaturated ketones afforded to corresponding Michael adducts with high enantioselectivity. The conjugate addition adducts are easily converted to chiral γ–keto nitroalkanes and γ–keto esters.



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Organocatalyzed intramolecular redox reaction via microwave irradiation: Synthesis of tetrahydroquinolines

권유경, 강영구, 김대영

순천향대 화학과

Tetrahydroquinolines have attracted considerable attention due to their diverse array of biological activities. Lewis acids, Bronsted acids and organocatalysts-mediated activation of unreactive C-H bond was recently reported.In this presentation, we wish to communicate organocatalyzed C-H bond functionalization via microwave irradiation. This synthetic method afforded high yields of tetrahydroquinoline derivatives with remarkably short reaction time than thermal experimental conditions.

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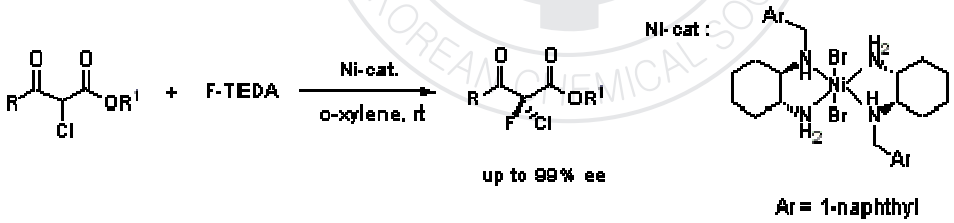
Catalytic Enantioselective Fluorination of α-Chloro-β-ketoester in the Presence of Chiral Nickel Complexes

강승희, 김대영

순천향대 화학과

Chiral organofluorine compounds containing a fluorine atom bonded directly to a stereogeniccenter have been utilized in studies of enzyme mechanisms and as intermediates in asymmetric syntheses. The catalytic enantioselective electrophilic fluorination promoted by chiral nickel complexes is described. The treatment of α-chloro-β-ketoesters with selecfluor under mild reaction conditions afforded the corresponding fluorinated α-chloro-β-ketoesters with excellent enantiomeric excesses (up to 99% ee).



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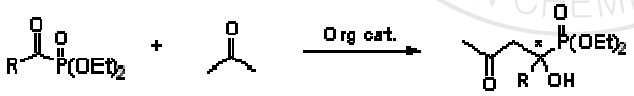
Enantioselective aldol reactions of α-keto phosphonates with ketones catalyzed by bifuntional organocatalysts

이현주, 김대영

순천향대 화학과

Chiral α-hydroxy alkylphosphonic acid derivatives have attracted extensive attention due to their excellent inhibitory bioactivities. It is well-known that, in a racemic mixture, normally only one enantiomer shows the observed activities, and therefore, an enantioselective method for the synthesis of these compounds is important. Herein we report the enantioselective synthesis of α-hydroxy alkylphosphates catalyzed by bifuntional organocatalysts. The treatment of α-keto phosphonates with ketones under mild reaction conditions afforded the corresponding tertiary α-hydroxy alkylphosphonates with high enantioselectivities (up to 93% ee).



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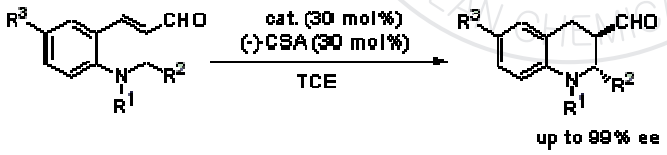
Enantioselective organocatalytic C-H bond functionalization via tandem 1,5-hydride transfer/ring closure

강영구, 김대영

순천향대 화학과

The development of C-H bonds functionalization has become an area of intense interest in synthetic organic chemistry because such reactions offer new strategies for the synthesis of complex organic targets. Lewis or Bronsted acids-mediated activation of unreactive C-H bond was recently reported. Herein we report the first organocatalytic enantioselective intramolecular 1,5-hydride transfer/ring closure reaction. This redox neutral reaction cascade allows for the efficient formation of ring-fused tetrahydroquinolines in high enantioselectivities (up to 99% ee).



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Design and synthesis of Simple Metallopeptide Sensor

김정민, Lohani Chuda Raj, 이건형

인하대 화학과

Recently, peptide probe sensors which work in aqueous solution have increased attention of the scientific community. We chose a fluorescent peptide sensor containing a dansyl fluorophore as a model peptide and investigated whether the selectivity and sensitivity of the peptides for heavy and transition metal ions could be tuned by change the length of ligand amino acids side chain. A new fluorescent peptide probe for the detection of Ag+ was synthesized in SPPS with Fmoc chemistry. The peptide sensor has a good solubility in aqueous buffer system; thus we investigated the fluorescence response to various metal ions in physiological buffer solution. Among the 14 metal ions, series of metallopeptide shows turn on response to Ag+ in 10 mM HEPES buffer solution (pH 7.4).

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Enantioselective Synthesis of Cyclic Sulfamidates by Chiral Rhodium-Catalyzed Asymmetric Transfer Hydrogenation

한주애, *강소영, **이은실, ***최은복, ****이현규

*과학기술연합대학원대 의약및 약품화학 *과학기술연합대학원대 의약 및 약품화학 **한국화학연구원 대사증후군치료연구 ***한국화학연구원 화학물질연구단 ****한국화학연구원 신약연구단*

Asymmetric transfer hydrogenation (ATH) of cyclic sulfamidate imines using HCO2H/Et3N mixture as hydrogen source and well defined chiral Rh catalysts (S,S)- or (R,R)-RhCl(TsDPEN)Cp*, (S/C=200~1000) effectively produced the corresponding cyclic sulfamidates with excellent yields and enantioselectivities at room temperature within 0.5 hr. ATH of 3,4-disubstituted imines having preexisting stereogenic center was shown to be accompanied by dynamic kinetic resolution.

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Dynamic Kinetic Resolution: Asymmetric Transfer Hydrogenation of 4,5-Disubsrituted Cyclic Sulfamidates Imines using Chiral Rhodium-Catalyst to Optically Active Cyclic Sulfamidates

한주애, *강소영, **이현규

*과학기술연합대학원대 의약및 약품화학 *과학기술연합대학원대 의약 및 약품화학 **한국화학연구원 신약연구단*

Dynamic kinetic resolution of 4,5-disubstituted cyclic sulfamidate imines via asymmetric transfer hydrogenation proceeded efficiently to give the corresponding cis-4,5-disubstituted cyclic sulfamidates with excellent yields and enantioselectivities at room temperature within 0.5 hr. Subjection of 4,5-diphenyl cyclic sulfamidate imine to HCO2H/Et3N mixture as hydrogen source and well defined chiral Rh catalyst, (R,R)-RhCl(TsDPEN)Cp*, at room temperature in either EtOAc or CH2Cl2 produced the corresponding (4S,5R)-diphenyl cyclic sulfamidate in 98% ee and 99% isolated yield.

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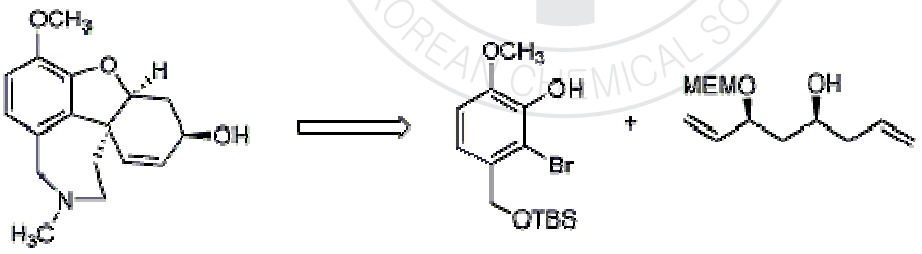
Synthetic Studies of (-)-Galanthamine

박상연, 태진성

연세대 화학과

The amaryllidaceae alkaloid (-)-galanthamine is a centrally acting acetylcholinesterase inhibitor and has found clinical use in the early treatment of Alzheimer's disease. We have studied asymmetric total synthesis of (-)-galanthamine starting from the known, enantiomerically pure epoxy alkenol generated by the Jacobsen's hydrolytic kinetic resolution (HKR) method. Mitsunobu reaction of an aryl alcohol and a dieneol was used to assemble the galanthamine backbone. The diene was cyclized using ring-closing metathesis and intramolecular Heck cyclization was utilized to set the cyclic ring system of galanthamine.



(-)-Galanthamine

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Sensing of specific ions by simple Rhodamine derivative and Calix[4]arene-TTF conjugates

이민희, 김종승

고려대 화학과

We prepared a new class of anion receptors bearing four tetrathiafulvalene (TTF) units at the upper rim of calix[4]arene linked through amid group and described its anion binding behaviors in organic solvent. In addition, two calix[4]arene-TTF conjugates in cone and 1,3-alternate conformations, respectively, were synthesized for comparative investigation to explore a tendency towards anion binding. The 1(cone) and 1(1,3-alternate) displayed broad absorption band at λ = 415 nm corresponding to the TTF units and showed brownish yellow color. From the absorption spectroscopic titration, the affinity order was as follows: 1(cone): $HP_2O_7^{3-}$ >$H_2PO_4^-$ >CH_3COO^- >F^- >Cl^-, 1(1,3-alternate): Cl^- >CH_3COO^- >$HP_2O_7^{3-}$ >$H_2PO_4^-$ > F^-. For further systematic study, the anion binding events were also investigated by monitoring ^{1}H NMR spectroscopy, and cyclic voltammetry (CV) in organic solvent.

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Selective hydrophobic derivatization on the surface of silica nanotubes

오채영, *김태규, 이미성, **문해경, 한현주, ***정의덕, 정옥상, ***진종성

*부산대 화학과 *한국기초과학지원연구원 **한국기초과학지원연구원 하이테크소재연구부 ***한국기초과학지원연구원 하이테크부품소재연구지원센터*

Helical mesoporous silica nanotubes bearing a gelator which is derivatized chiral 1,2-diphenylethylenediamine were prepared through the sol-gel polycondensation of TEOS by using organogels as templates. The selective hydrophobic functionalization on the surface of mesoporous silica nanotubes could be achieved by a post-graft method. Also, we have confirmed to the derivatization on the surface of mesoporous silica nanotubes by using analysis of high performance liquid chromatography (HPLC), thermogravimetric analyzer (TG) and elemental analyzer (EA).

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Turn-On Fluorescence Sensing of Cysteine

정효성, *강철훈, **이진용, 김종승

*고려대 화학과 *경희대 동서의학대학원 **성균관대 화학과*

The new coumarin-based chemodosimeter effectively and selectively recognizes cysteine over the structurally similar homocysteine and glutathione, based on a Michael type reaction. From the TDDFT calculations, fluorescence amplification of probe upon reaction with cysteine is due to an ICT blocking event. Cysteine selectivity of probe over homocysteine and glutathione was also proven by LC-MS spectroscopic methods using the metabolite from the HepG2 cell line. From the confocal microscopic study, probe showed marked fluorescence enhancement for cysteine over other thiol functionalized amino acids. Its selective reactivity toward cysteine over other thiol containing species was presumably due to the lower pKa value for its thiol unit than those of other thiols, as well as steric effects. It is thus the contention of the authors that this novel finding would be an important guideline in designing fluorescent turn-on sensors for the biologically relevant amino acid, cysteine.

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Synthesis of mono-cyclic natural compound with controlled cyclization reaction

서정아, *구상호

*명지대 나노공학과 *명지대 화학과*

Cyclic structures are prevalent in biologically important natural products therefore, the development of efficient cyclization method is very important in organic synthesis. We've discovered that the cyclized products with the internal sulfone group can be efficiently used in the synthesis of various natural products. This study includes efficient synthesis of mono-cyclic natural compound with isoprenoid chain containg sulfone group.

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Synthesis of various substituted Unnatural Carotenoid via conjugated allylic sulfones

임보람, 오은택, *구상호

*명지대 나노공학과 *명지대 화학과*

In terms of stability and electronic characteristic, the conjugated polyene chains of unnatural carotenoids containing aromatic substituents compared with that of the natural carotenoids. The unnatural carotenoid can be divided to 2 parts; allylic sulfone containing various substituents and dial unit. Of this, allylic sulfone unit is used useful material in the diversely substituted synthesis of carotenoid compound. The homoallylic alcohol containing homoallylic sulfone moiety can be prepared by the Indium-mediated addition haloallylic sulfone to aldehyde. The reaction provides high stereoselectivity as well as an absolute regioselectivity. and the selectivity is originated from the substituents; Me group to anti selectivity and Ph group to syn selectivity. This homoallylic alcohol produces the allylic sulfone containing a conjugated polyenes by the Oxonia-Cope rearrangement.

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A Highly Efficient Synthetic Method of Oxy-carotenoid Compounds

심상은, *구상호

*명지대 나노공학과 *명지대 화학과*

We have reported an efficient synthetic methods of carotenids based on the sulfone coupling and double elimination strategy using C20 dialdehyde ((2E,6E,10E,14E)-2,6,11,15-tetramethyl-8-(phenylsulfonyl) hexadeca-2,6,10,14-tetraenedial) and C10 sulfone unit (((2,6,6-trimethylcyclohex-1-enyl)methylsulfonyl) benzene). Oxy-carotenoids are prepared by coupling of oxidized C10 sulfone unit and C20 dialdehyde. This study includes controlled oxidation of C10 sulfone unit and its coupling, protecting and double elimination with C20 dialdehyde.

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Synthetic method of various carotenoid as the nano wire

김형준, *구상호

*명지대 나노공학과 *명지대 화학과*

The carotenoids are an important class of organic molecules with delocalized π-electrons. We have perfectly 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, the allylic sulfone containing aromatic substituents and dialdehyde, for the systematic construction. These two subunits can be disconneted 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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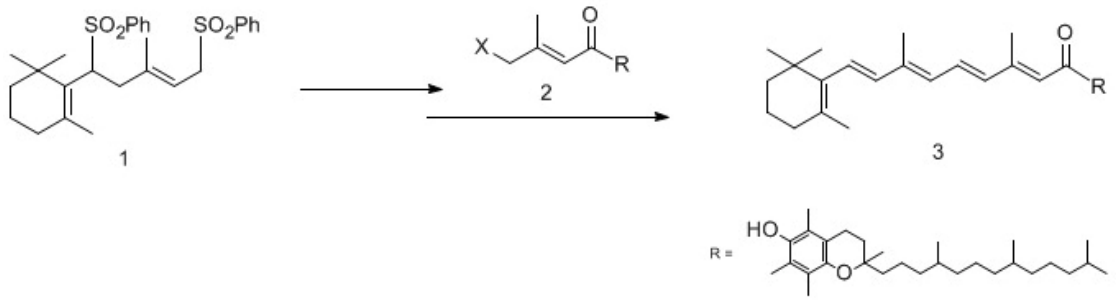
Study on The New Synthetic Method : Retinoic acid Derivatives Tocoretonate

오은택, *구상호

*명지대 나노공학과 *명지대 화학과*

We have efficiently synthesized retinoic acid derivatives containing Tocopherol moiety. This procedure involves coupling of C15-disulfone 1 and C5-Ester bromide 2 containing tocopherol followed by desulfonation reaction. Unit(1) was prepared from geranyl Sulfone and unit(2) was prepared from 3,3-dimethylacrylic acid with Tocopherol by the Esterification. Synthesis and result will be discussed in detail.



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The Methodology and Applications of Selective Reduction of Allylic Alcohols

Liang Su

명지대 화학과

Several kinds of reactions can result in the synthesis of allylic alcohol products. Becauses of its prevalent in existence, people who work in organice synthesis field are trying to find a good series of methods for controlling this kind of compounds. We have developed our selective reduction method of allylic alcohols by the formation of 1-alkoxyallyl ethers and Pd-catalyzed Super Hydride reductionsequence. And it is very interesting from a mechanistic as well as synthetic viewpoint. Our method has great advantage especially when allylic alcohols which containing a non-activated alcoholic moiety at the same time. The selectivity of our method help us to be able to make some difficult stuctures and it has already be applied in the total synthesis of Lavandulol. Furtherapplications and the details will be discussed during the presentation.

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Synthesis of Retinoic acid derivatives and Self-assembling properties of Retinyl Ethers

박선영, *구상호

*명지대 나노공학과 *명지대 화학과*

Retinoic acid is a nutrient that body needs in small amounts to function and stay healthy. We developed effective and practical method for preparing retinoic acid, retinoic acid derivatives by using C_{15}-monosulfone and various C_5-units compound, that is prepared through allylic halogenation. We found a synthetic method of retinyl ethers from various alcohols. The retinyl ether of amino acid tyrosine were self-assembled and showed an interesting morphology depending on the solvent used for extraction. The morphology and structure of the retinyl ether were analyzed by scanning electron microscope.

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The intramolecular reductive cyclization of alkyne-aldehyde

강민정, 홍종태, 장혜영

아주대 에너지시스템학부

The reductive cyclization of alkyne-aldehyde is a typical reaction to form a ring structure which is abundant in natural products. In this presentation, a Pt complex genarated from $PtCl_2$, $SnCl_2$, and phosphine ligand was applied to the cyclization of alkyne-aldehyde to provide the desired cyclization product. For the optimization of the reaction conditions, various substrates and phosphine ligands were examined. It was found out that the Pt catalyst possessing electron-rich ligands favors the reductive cyclization while an electron-deficient Pt complex prefers the heteroenyne metathesis route. In addition, the functional groups and length of the substrates are important factors for reductive cyclization.

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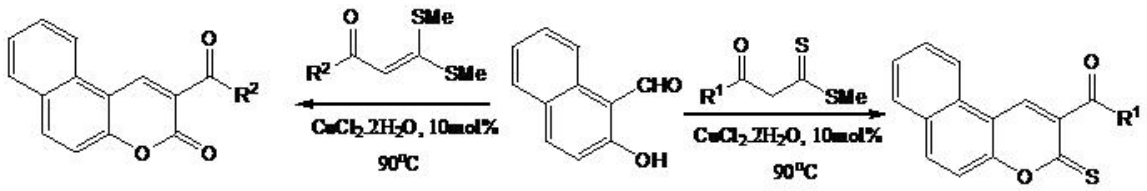
Facile Synthesis of 3-thioxo-3H-benzo[f]chromen-2-yl methanone and 3H-benzo[f]chromen-3-one under solvent free condition

임기범, 김현진, 김민규, 이상경

경상대 화학과

Many classical routes have been available for the synthesis of coumarin. The Pechmann reaction for the synthesis of coumarin involves the condensation of phenols with β-ketonic esters in the presence of variety of acidic condensing agents such as sulphuric acid, hydrochloric acid and phosphoric acid, phosphorous pentoxide, trifluoroacetic acid and Lewis acids such as ZnCl2, AlCl3 and exchange resins, have also been used.We have successfully demonstrated the facile synthesis of two different coumarin derivatives by the reaction of 2-hydroxy-1-naphthaldehyde with easily accessible β-oxodithioester and S,S-acetal in the presence of catalytic amount of CuCl2 under solvent free condition. This scheme offers a good scope for the synthesis of a wide variety of coumarins.



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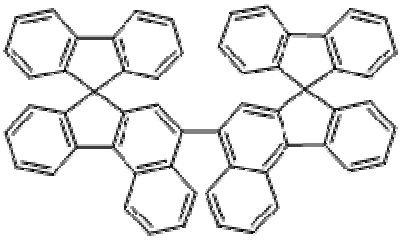
Spiro[fluorene-benzofluorene] 이량체 유도체들의 합성 및 광학적 특성조사

서정아, 김지영, 이인호, 공명선

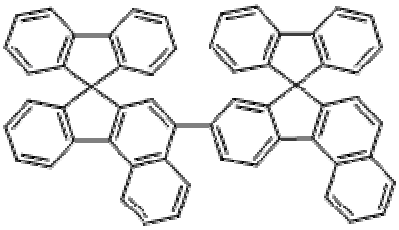
단국대 나노바이오의과학과

최근 OLED 용 도판트 및 호스트 재료에 많이 응용되고 있는 spiro[fluorene-benzofluorene]을 이용하여 새로운 형태의 spiro series, SM1-1, 2, 3 과 SM2-1, 2, 3 이라 명명한 dimeric spiro[fluorene-benzofluorene]유도체들을 합성하였다. 이러한 spirobenzofluorene 들은 높은 유리전이 온도와 높은 융점을 가지기 있으며 무결정이기 때문에 organic glass 라 불리우기 때문에 이러한 spirobenzofluorene 단위를 모체의 여러 위치에 치환하여 새로운 기능을 가지는 형광체로서 기대된다. 그 구조를 1H-NMR 과 13C-NMR, GC-Mass, 원소 분석을 통하여 분석 확인하였으며 또한 DSC 및 TGA 로서 열적성질, UV, PL, HOMO, LUMO 및 PL efficiency 등의 광학적 특성을 조사하였다.

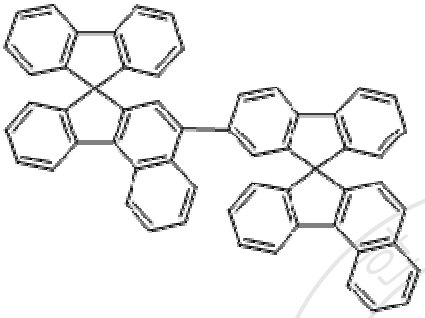
*** spiro-spiro scheme**



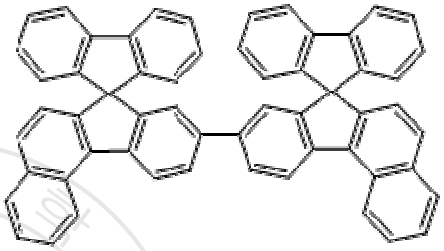
SM1-1



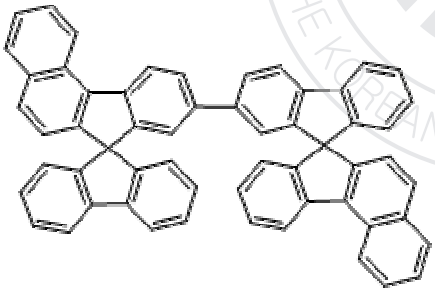
SM1-2



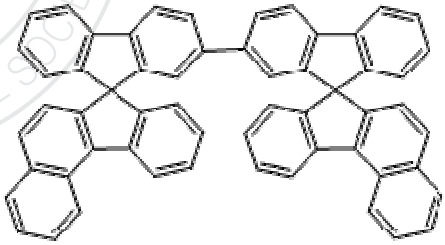
SM1-3



SM2-2



SM2-3



SM3-3

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Pt-Catalyzed Hydrogenation of Allene-carbonyls and Allene-imines

김지환, 홍종태, 장혜영

아주대 에너지시스템학부

The reductive cyclizations of the allene-carbonyl and allene-imine were studied under environmentally benign hydrogenation conditions. The cyclization was explored by using a Pt catalyst generated from $PtCl_2$, $SnCl_2$, phosphane and H_2. The catalytically competent platinum-hydrides react with allenes via hydrometalation, affording allylplatinum intermediates. The allylplatinum complexes were added to the carbonyl and imine moieties, providing synthetically versatile cyclic homoallylic alcohols and amines in reasonable yield. Deuterium labeling studies confirmed the occurrence of a allylplatinum formation from a Pt–hydride complex and the allene.

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Facile synthesis of fused-triazole compounds from the oxidative cyclization of heterocyclic hydrazones using Ca(OCl)2/Al2O3

송양헌, 황지나

목원대 화학과

Various fused-triazole compounds and new 3,7-diphenylthieno[3,2-e]bis[1,2,4]triazolo[4,3-a:4',3'-c]pyrimidine derivatives were easily synthesized at room temperature in good yield by the oxidative cyclization of heterocyclic hydrazones or thienopyrimidinyl hydrazones with alumina-supported calcium hypochlorite (Ca(OCl)2/Al2O3).The advantage of our protocol is easy workup, mild reaction conditions, fast reaction rates, and good yields, which make the method a useful contribution to the present methodologies.

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Hydrogen-Mediated Reductive Cyclization of Allenynes;Hydrometalation Susceptibility of Alkynes versus Allenes

김효동, 장혜영

아주대 에너지시스템학부

Pt complexes were used in the presence of phosphine ligands, $SnCl_2$, and H_2 for the cyclization of nitrogen-, carbon- and oxygen- tethered allenynes providing five- and six-membered cycloreduction products in good yield. By screening various phophine ligand it was found out that electron-rich phosphine gave the best yield. Based on deuterium labeling study, there are two possible ways for the hydrometalation of allenynes. To probe the working mechanism, various control experients were conducted. This study is expected to contribute to the design and development of efficient and versatile Pt catalysts for a wide variety of hydrogen-mediate reductive coupling reactions

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A Synthesis of 2-Guanidyl-1,3-thiazoles as Novel T-type Calcium Channel Blocker

허정회, *남기달, *신동윤, 정낙철, *한호규

*고려대 화학과 *KIST 생체과학연구부*

T-type channels are distinguished among voltage-gated Ca^{2+} channels by their low voltage thresholds. T-type Ca^{2+} channel is known to relation with hypertension, angina pectoris, epilepsy, cancer and neuropathic pain. We reported that 2-imino-1,3-thiazolines showed T-type Ca^{2+} channel inhibitory property. In the course of an exploration of novel T-type Ca^{2+} channel inhibitor we have designed new 2-guanidyl-1,3-thiazole derivatives by molecular modification of the 2-imino-1,3-thiazolines. The 2-guanidyl-1,3-thiazole derivatives have 1,3-thiazole and guanidyl moities within a molecule. 1,3-Thiazole is known to privileged scaffold and guanidyl group is emerging as a useful class of moiety, due to their interesting electronic properties and the capacity for facile derivatization. The target compounds were synthesized by the condensation of guanidylthiourea with various α-halo ketones. The synthetic route and their screening results will be presented.

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Novel 2-Amino-1,3-thiazoles as Suppression of Glutamate-Induced Excitotoxicity

한영휘, *남기달, *신동윤, 이덕형, *한호규

*서강대 화학과 *KIST 생체과학연구부*

Glutamate is one of the most abundant free amino acids in the central nervous system and is thought to be a major excitatory neurotransmitter. We reported a glutamate-induced excitotoxicity of 2-imino-1,3-thiazoline derivative. As an extension of our study on the development of new pharmaceuticals that useable for neurodegenerative diseases a group of 2-amino-1,3-thiazoles were synthesized. 2-Amino-1,3-thiazole is known to be privileged structure and a isoform of the 2-imino-1,3-thiazoline. Over thirty compounds were synthesized to establish the structure-activity relationship of 2-amino-1,3-thiazole derivatives. The synthetic pathway and the results of the biological activity against glutamate induced excitotoxicity will be presented.

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Na+ binding with azacrown induced changes of electrochemical and photophysical properties in Alkynylpyrene

배창완, 김종승

고려대 화학과

The 1,3,6,8-tetraethynylpyrene incorporating four 1-aza-15-crown-5 ether moieties has been synthesized to show unique patterns in photophysical and electrochemical properties in the presence of specific metal ions. The 1-aza-15-crown-5 ether unit is capable of binding Na+ ion effectively, which can induce changes of emission intensity and radical stability in pyrene platform. In addition, for further application such as organic light-emitting, ECL (Electrogenerated chemiluminescence) experiment are in progress upon the addition of Na+ ion.

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Catalytic Reductive Cyclization of alkyne-alkenes and alkyne-dienes

Wang Xi, 장혜영

아주대 에너지시스템학부

Transition metal-catalyzed cyclization reactions have emerged as extremely attractive and unique tools for the synthesis of various types of cyclic compounds. Among the transition metal complexes used for such transformations, Pt complexes has been implemented as a powerful strategy for the cyclization of alkyne-dienes and alkyne-alkenes. The new catalytic systems involving Pt(II) and SnX_2 to promote alkyne-dienes and alkyne-alkenes cyclizations have been studied. This catalytic system produced 5-memberd ring cycloreductions products in moderate to good yields by using carbon- and nitrogen-tethered substrates.

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Spiro[fluorene-7,9′-benzofluorene] host materials for blue light-emitting electroluminescence device

전영민, *이인호, *공명선

*단국대 화학과 *단국대 나노바이오의과학과*

진한 청색 계열의 형광을 띠는 스피로 형태의 호스트로서 5,9-di(naphthalen-2-yl)spiro[benzo[c]fluorene-7,9'-fluorene] (BH-6NSP), 5,9-bis(4-t-butylphenyl)spiro[benzo[c]fluorene-7,9'-fluorene] (BH-6tBSP) 그리고 5,9-bis(4-fluorophenyl)spiro [benzo[c]fluorene-7,9'-fluorene] (BH-6FSP)인 BH-6 계열 3 종을 합성하였다.LED 소자 응용 평가를 위한 다층 구조는 ITO / N,N'-diphenyl-N,N'-bis[4-(phenyl-m-tolyl-amino)phenyl]biphenyl-4,4'-diamine(DNTPD)/N,N'-di(1-naphthyl)-N,N'-diphenylbenzidine(NPB)/Host:BD-6DPA/tris(8-hydroxyquinoline)aluminum (Alq3)/LiF 와 위 소자에 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline(BCP) 재료 하나를 더 추가하여 2 가지 형태의 소자 제작을 하였다. dopant 재료로서는 기존의 합성되어진 N,N,N',N'-tetraphenylspiro[benzo[c]fluorene-7,9'-fluorene]-5,9-diamine (BD-6DPA)를 사용하였으며 전기/광학적 평가, EL 발광스텍트럼, CIE 색좌표 등을 이용하여 소자의 평가를 실시하였다.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Pt-catalyzed reductive cyclization of Alkyne-hydrazones

오현지, 장혜영

아주대 에너지시스템학부

The reductive cyclization of alkyne-hydrazones was studied under environmentally benign hydrogenation conditions. A nitrogen-tethered alkyne-hydrazone efficiently undergoes Pt-catalyzed reductive cyclization to afford a five-membered ring bearing a protected amine and vinyl phenyl functionality. To conduct such transformation, Pt(Ⅱ) catalysts were applied in the presence of phosphines, $SnCl_2$ and H_2. For the optimization of the reaction conditions, several phosphine ligands and additives were applied. While cyclizations of alkyne-aldehydes were actively investigated, there are only a few examples of alkyne-imine derivatives cyclization. In this paper, we describe an optimization and the substrate scope of a new synthetic cyclization protocol under environmentally friendly hydrogenation conditions.

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Thiazole-based chemosensor : synthesis and fluorescence sensing of $CH_3CO_2^-$

Aasif Helal, 김상현, 김현곤, 김홍석

경북대 응용화학과

Novel fluorogenic sensors based on urea derivative of 2-(2'-aminophenyl)-4-phenylthiazole (4 and 5) were prepared and used for recognition of anions with similar basicity and surface charge density. Chemosensor 4 was found to be highly selective to acetate ion over other anions. The selectivity was related to the structure matching between the host and the guest. The evaluation of the chemosensors interaction with anions was performed by UV-vis and fluorescence titration. This acetate binding affinity was further tuned by varying the acidity of the N-H proton of the urea moiety in chemosensor 5.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Thiazole – sulfonamide based chemosensor:synthesis and ratiometric fluorescence sensing of zinc

Aasif Helal, 김상현, 김현곤, 김홍석

경북대 응용화학과

A new thiazole-sulfonamide (ATP, 1) based zinc selective emission ratiometric probe suitable for biological applications in aqueous ethanol, was synthesized and investigated. The mechanism of fluorescence was based on the cation-induced inhibition of excited-state intramolecular proton transfer (ESIPT).

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Molecular recognition of carboxylic acid through fluorescence excimer formation by cholesterol based imidazolium receptor

Md. Wasi Ahmad, Jadav Jyoti, 김홍석

경북대 응용화학과

A novel cholesterol-based fluorescent chemosensor has been designed and synthesized, where the imidazole is used as the binding site and the pyrene as the fluorophore. Carboxylic acids are the most attractive targets for molecular recognition. Receptor 1 shows enhanced excimer emission fluorescence in ethanol towards oxalic acid.

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Copper(I)-Catalyzed Regio-and Stereoselective Boron Addition to Internal Alkynes

김혜령, 채동훈, 윤재숙

성균관대 화학과

The boration of alkynes is a useful method for the preparation of alkenylboron compounds, which are versatile organic building blocks in organic synthesis. We attempted to develop better catalytic systems for the regioselective synthesis of alkenyl boron compounds with use of diboron reagents. So we developed the efficient monophosphine-copper catalytic system that allows highly regio-and stereoselective boron addition to internal alkynes to form (Z)-alkenylboronates in the presence of methanol. These alkenyl boronates are useful intermediates for the stereospecific synthesis of various diarylalkens which are useful synthesis of natural products and pharmaceuticals.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Application of Dibenzothiophene Moiety for Organic Light Emitting Materials

박영진, *한우택, *황선우, *박은랑, *이상우, *김인태

*광운대 화학과 고분자연구실 *광운대 화학과*

Recentyl, novel materials from dibenzothiophene-S,S-dioxide moiety for OLED have been designed and synthesized. Then we introduced alkoxy group as solubility, electron donating effect and fluoro group as electron withdrawing effect on dibenzothiophene moiety. The structure of the resulting compounds were characterized by ^{1}H NMR, ^{13}C NMR and FT-IR. The optical properties and electronic properties of the resulting compounds were measured by UV-vis spectroscopy and cyclovoltammetry, respectively. The new materials were applied to OLED as emitting materials.

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Synthesis and Characterization of Well Defined EDOT Containing Hetero Aromatic Oligomers

한우택, 박은랑, 김인태

광운대 화학과

Thiophene based contain EDOT 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 synthesised novel oligomer compounds EDOT. 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.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Synthesis of Diphenylamino Substituted Quinoline (acceptor) and Thiophene (donor) Based Organic Dyes for Solar Cells

조정임, 권태우, 안택

경성대 화학과

New organic dyes that contain diarylamino substituted quinoline and thiophene moiety have been synthesized. As a key intermediate in the synthesis of organic dyes for solar cell applications, we have designed the diarylamino benzophenone containing the diphenylamino moieties. Aldehyde-functionalized thiophene was introduced via Suzuki coupling reaction between bromide(4-(6-bromo-4-phenylquinolin-2-yl)-N,N- diphenylbenzenamine)and boron(5-formylthiophen-2-ylboronic acid). Vinylene linkages having CN and COOH functional group were also achieved by using a Knoevenagel reaction. The chemical structures of synthesized organic dyes were characterized using 1H, 13C-NMR and FT-IR spectrometer. In addition, the optical properties of novel organic dyes were investigated by UV-visible absorption and photoluminescence measurement as solution and thin-film state. Detailed synthetic schemes and characterizations of new donor-acceptor combined organic dyes will be presented.

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Synthesis of 1H-2,3,1-Benzothiadiazine-2,2-dioxides using N-t-Butyloxycarbonyl-N`-arylsulfamide as Potential BNCT Agent

임현화, 이채호, *강상욱, **이종대

*원광대 생명나노화학부 *고려대 소재화학과 **조선대 화학과*

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). 4-Carboranylmethyl-1H-2,1,3-benzothiadiazine-2,2-dioxides 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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Uridine-based Paramagnetic Amphiphiles: First Examples of Nucleoside-based Potential T1 MRI Contrast Agents

이수민, 김종승

고려대 화학과

Magnetic resonance imaging (MRI) is a powerful noninvasive technique that provides high quality three dimensional images of soft tissues, including information on anatomy, function, and metabolism of tissue in vivo. MRI contrast agents (CAs), in particular gadolinium-based agents, are safe and lack the nephrotoxicity associated with iodinated contrast media. The chelated Gd3+ metal ion improves imaging contrast by increasing the longitudinal relaxation time (T1) of proximal water protons, which appear brighter in the T1-weighted image.Recently, this lab has synthesized for the first time uridine nucleoside-based amphiphilic gadolinium complexes as MRI contrast agents. The highest relaxivities achieved were 30.3 and 22.6 mM-1s-1 in PBS solution (pH 7.4) at 0.47 and 1.41 T, respectively, for LGd3. The new complexes demonstrated binding affinity towards HSA with further enhanced relaxivity. Most importantly, the pH dependent relaxivity change of LGd3 encouraged use in pH mapping of tissue. Stability studies of the complexes against transmetallization with Zn2+ indicated that these new amphiphilic complexes are quite stable and comparable with clinically used Magnevist® and Omniscan®. LGd3 is the first example of a self-assembled paramagnetic amphiphilic with high relaxivity, HSA binding ability, and pH response among other reported amphiphilic gadolinium-based contrast agents.

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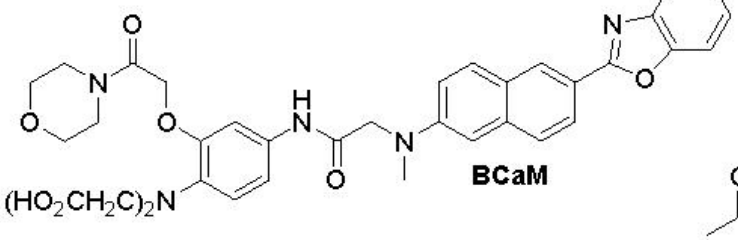
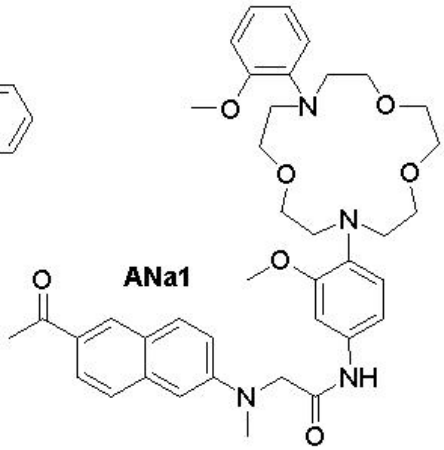
Dual-Color Imaging of Sodium/Calcium Ion Activities with Two-Photon Fluorescent Probes

김형중, *한지희, 김미경, **임창수, 김환명, **조봉래

*아주대 에너지시스템학부 *고려대 화학 **고려대 화학과*

Calcium is a ubiquitous second messenger controlling numerous cellular functions. Intracellular free Ca^{2+} concentrations are maintained by the coordinated actions of various calcium channels and transporters, including the Na^{+} /Ca^{2+} exchangers (NCX), which transports one Ca^{2+} out of the cell and take three Na^{+} ions into the cell. Herein, we report a TP probe (BCaM) that shows a 14-fold two-photon excited fluorescence (TPEF) enhancement in response to Ca^{2+}, intracellular dissociation constant of 78 μM, high sensitivity and selectivity for near-membrane Ca^{2+} ions. Superior to currently available probes, this probe, in combination with ANa1, allows dual-color imaging of the activities of near membrane Ca^{2+} and cytosolic free Na^{+} ions in live cells and tissues at depths > 100 μm for long periods of time without artifacts of photobleaching.





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Multi-Color Emissive Two-Photon Dyes for Specific Applications

MASANTA GOUTAM, *박선근, **임창수, **조봉래, *김환명

*아주대 분자과학기술연구센터 *아주대 에너지시스템학부 **고려대 화학과*

Two-photon microscopy (TPM) has become an indispensible tool in biology and medicine due to the capability of imaging the intact tissue for a long period of time. To make it a versatile tool in biology, a variety of two-photon probes for specific applications are needed. Combined with appropriate two-photon (TP) probes, TPM can image deep inside the intact tissue for a long period of time. However, the progress in this field is hindered by the lack of TP probes for specific applications. Moreover, most of the OP fluorescent probes used for TPM have low TP cross sections (δ_{TPA} < 50 GM) that limit their use in TPM. Herein, we describe a series of two-photon multi-color emissive dipolar molecules for various TP probes. These compounds can be easily synthesized, show appreciable water solubility, and emit strong two-photon fluorescence in the physiological condition.

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Visualization of Intracellular Sodium ion with Two-Photon Probes

김미경, *한지희, **조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학 **고려대 화학과*

Sodium ion plays critical roles in many physiological and pathological processes. Very recently, we reported a two-photon (TP) probe (ANa1) that shows strong TPEF enhancement in response to Na^+, a dissociation constant of 26 mM in the cell, can be easily loaded into the cells, emits 3~5-fold larger TPEF than commercially avalible probes upon complexation with Na^+, and can selectively detect $[Na^+]_i$ in live cells and living tissues at 100-200 μm depth for more than 60 min using TPM. However, there is no report on the organelle-specific TP probe for Na^+ ion. Herein, we report the design, synthesis, and bioimaging applications of a new type TP probe (1) for detection of mitochondrial Na^+ ions.

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Development of Two-Photon Probes for Imaging Zinc Ion in Vivo

MASANTA GOUTAM, *백나영, **임창수, **조봉래, *김환명

*아주대 분자과학기술연구센터 *아주대 에너지시스템학부 **고려대 화학과*

Zinc ion is an essential component of many enzymes and proteins. In the brain, a few millimoles of intracellular free Zn^{2+} ions are stored in the presynaptic vesicles, released with synaptic activation, and seem to modulate excitatory neurotransmission. Design of two-photon (TP) fluorescent probes which allow visualization of cations, small molecules, or enzyme activity in living cells by two-photon fluorescence microscopy (TPM) are of current intereset. However, efficient two-photon probes for Zn^{2+} are still demanding. To address this problem, we designed two-photon probes (1 and 2) that show > 40-fold two-photon fluorescence enhancement and bright TP excited fluorescence in response to Zn^{2+}, sufficient water solubility, high selectivity for Zn^{2+} ions, pH resistance, and high photostability. We also designed a new type TP probe (2-Mito) for selectively detection of mitochondrial Zn^{2+} ions in vivo.

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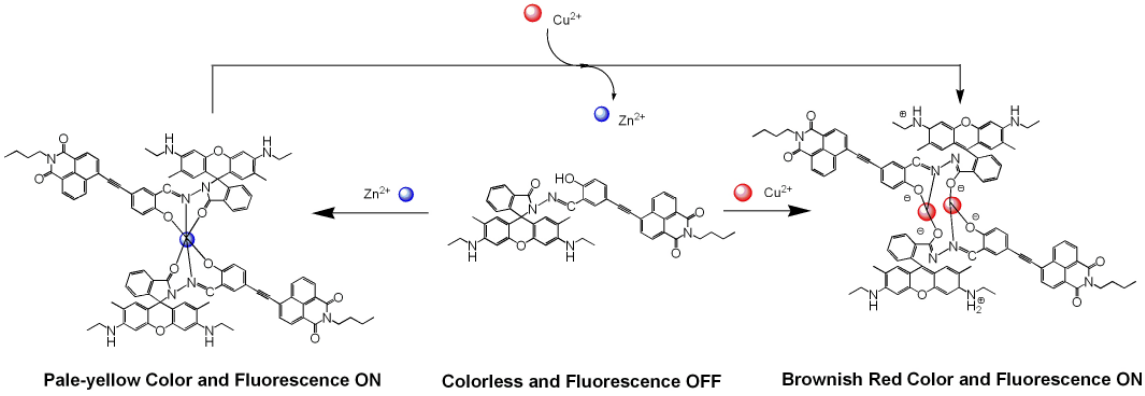
Naphthalimide Modified Rhodamine Derivative: Ratiometric and Selective Fluorescent Sensor for Cu2+ based on Two Different Approaches

ZHANG JUNFENG, 김종승

고려대 화학과

Fluorescent sensors for the detection and measurement of transition-metal ions are widely investigated because of their simplicity and high sensitivity of response. In particular, the development of a fluorescent probe for copper ions in the presence of a variety of other metal ions has received great attention.We recently reported a novel fluorescent sensor 1, which showed a ratiometric and 'off-on' response to Cu2+ based on rhodamine ring-opening approach. Moreover, the 1-Zn2+ can be displaced by Cu2+, which resulted in another ratiometric sensing signal output. Thus, 1 can be a dual mode Cu2+-selective sensor via the rhodamine ring-opening mechanism and ratiometric displacement mechanism. Remarkable fluorescence enhancements were detected upon the addition of Zn2+ and Cu2+, respectively. Upon binding Zn2+, 1 showed a broad emission band centered at 595 nm, which is similar as excitation at 400 nm, implicating that a promoted ICT process occurred. In contrast, upon binding Cu2+, only enhanced fluorescent intensity at 550 nm were observed, suggesting that sensor 1 recognizes Cu2+ principally based on the rhodamine ring-opening mechanism. The increases of absorbance and fluorescence intensity resulting from the addition of the Cu2+ ion were not influenced by the subsequent addition of miscellaneous cations. All these indicate that the selectivity of 1 for the Cu2+ ion over other competitive cations in the water medium is remarkably high.



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Multi porphyrin dendrimer for supramolecular assembly

이도형, 장우동

연세대 화학과

Host-guest chemistry, an important part of supramolecular chemistry, describes a chemistry that held complexes composed of more than two molecules with unique site-specific binding properties where the force that makes host-guest complex is noncovalent bonding, such as hydrogen bonding, metal coordination, π-π interation, and van der Waals force. Recently, several porphyrin-based host-guest chemistry studies have been reported, for the design of artificial light harvesting, self-assembly, and site-selective catalyst. It is known that zinc porphyrin works as a Lewis acid by accepting axial ligands which has electron lone pair. For instance, some researchers found that 5,10,15,20-tetra(4-pyridyl)porphyrin(TPyP) can bind to zinc porphyrins. Also this property can be applied to energy transfer, which can occur from zinc porphyrin to free-base porphyrin. To expand these porphyrin properties, we designed a multi-porphyrin dendrimer which expects to bind TPyP. By UV-Vis, FL-titration and Job`s plot, we assume that one multi porphyrin dendrimer can accomodate two TPyP molecules. Also, FL-titration shows that when TPyP binds to porphyrin assembly, energy transfer occurs from porphyrin assembly to TPyP.

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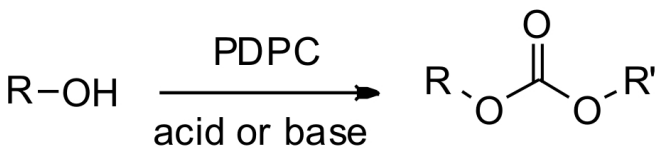
Synthesis of Organic Carbonate with Phenyl 4,5-Dichloro-6-Oxopyridazine-1(6*H*)-Carboxylate

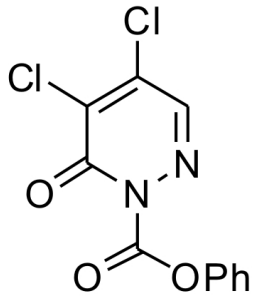
김은정, 김보람, 이인혜, *김점종, 윤용진

*경상대 화학과 *한국전자통신연구원 차세대태양광연구부*

Organic carbonates have played very important roles for the synthetic intermediates of fine chemicals, pharmaceuticals, plasticizers, synthetic lubricants, and monomers for organic glasses. They are also used in organic reaction as solvents. Although some methods reported, these require special additives, and also CO, CO_2 and hazardous phosgene as a carbonyl source. Recently, we developed phenyl 4,5-dichloropyridine-1(6*H*)-carboxylate as carbonyl source. Herein, we present convenient method of organic carbonates from alcohols using phenyl 4,5-dichloropyridine-1(*6H*)-carboxylate.



R = Alkyl, aryl R' = Alkyl, aryl



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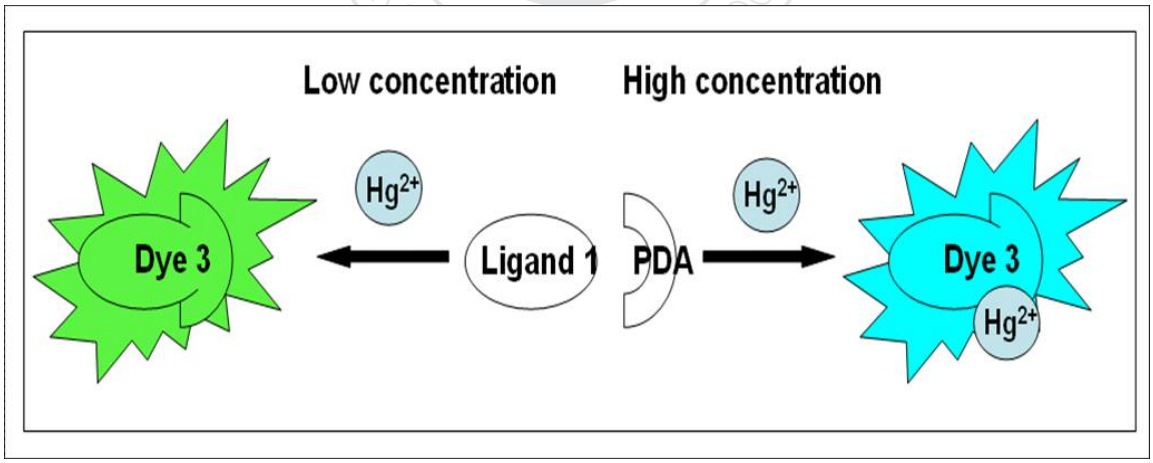
발표종류: 포스터, 발표일시: 목 10:30~12:30

A new fluorogenic chemodosimetric system for mercury ion recognition

임문수, 김종승

고려대 화학과

A new probe system for fluorogenic sensing of mercury ions has been designed and synthesized. It is the first intermolecular reaction-based fluorogenic chemodosimetric probe system for Hg(II) ion recognition. High and low concentrations of mercury ions gave different fluorescence responses that could easily be distinguished by the naked eye. This unique system allows detection of the concentration and presence of the mercury ion.



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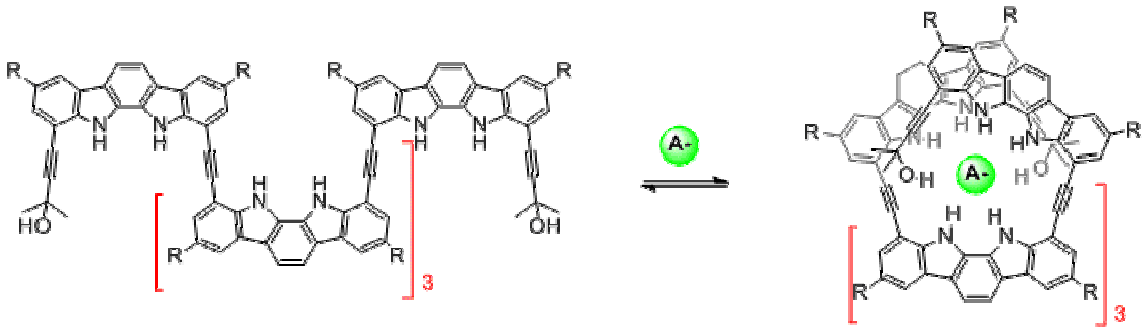
Indolocarbazole pentamer as an anion receptor

김민정, 정규성

연세대 화학과

Indolocarbazole is an aromatic heterocycle that contains two built-in NH protons in a convergent manner and therefore forms strong hydrogen bonds with ions and molecules. In recent years, we and others have demonstrated that the indolocarbazole unit can serve as a useful building block to construct various types of anion receptors such as molecular clefts, macrocycles and acyclic oligomers. Herein, we prepared an indolocarbazole pentamer that consisted of five indolocarbazole units linked through ethynyl bridges and of two propagyl OHs at ends. The pentamer possesses twelve hydrogen bond doners, 10 NHs and 2 OHs, thus being able to strongly and selectively bind anions of complementary size, shape and hydrogen bonding mode. Details will be described in the presentation, including structures and anion-binding properties.



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Nitration of disubstituted aromatic compounds using NH_4NO_3 and their application to organic intermediate synthesis

박희근, 박균하

충남대 화학과

Nitration of aromatic compound is an industrially important reaction since the nitrated products are intermediates for chemical industries and pharmaceuticals. However, reaction of using HNO_3 is notorious for several reasons, such as safety concerns and generation of impurities due to oxidation. To solve this problem, various nitration of substituted aromatic compounds was achieved employing NH_4NO_3 and acid catalyst in $CHCl_3$ or CH_3CN. This protocol provides most convenient and reliable way for nitration. Based on the experimental results valuable intermediates were synthesized and these will have wide application to build up structures.

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Development of Synthetic Method of Multi-Substituted Coumarins

김현석, 박성국, 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 and 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. Coumarins have been synthesized by several routes including Pechmann, Perkin, Knoevenagel, Reformatsky and Wittig reactions. 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 H_2SO_4, $FeCl_3$, $ZnCl_2$, $AlCl_3$ and HCl are all well documented in the literature. In this poster, we report new synthetic method of coumarin derivatives.

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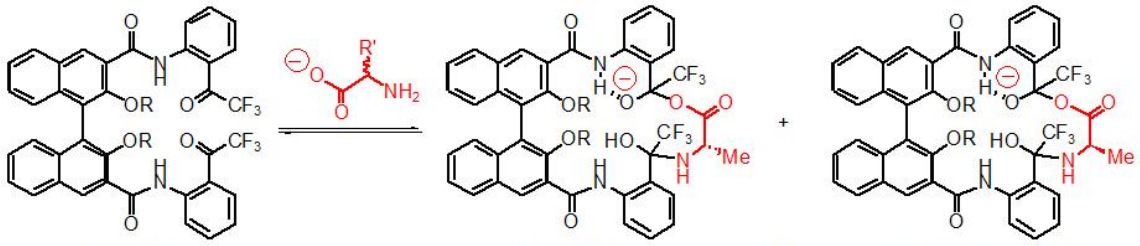
Chiral Discrimination of α-aminoacids with C2-Symmetric Homoditopic Receptor

sunderraman

포항공과대 화학과

한국화학회 THE KOREAN CHEMICAL SOCIETY

Sunderraman Sambasivan, Dae-Sik Kim and Kyo Han Ahn*Department of Chemistry and Center for Electro-Photo Behaviours in Advanced Molecular Systems, Pohang University of Science and Technology, Pohang, 790-784, Republic of Korea.E-mail : ahn@postech.ac.krMost of the α-amino acid chiral receptors developed hitherto, contain different binding moieties for the recognition of the amine and the carboxylate groups. One major consequence of using different binding moieties is that the chiral receptor so designed, loses its symmetry. The importance of symmetry in a chiral receptor or catalyst, is well documented. Molecular symmetry can reduce the number of possible intermediates or transition states and hence dramatically increase the probability of success in chiral recognition or in asymmetric reaction catalysis, as the case may be.A C2-symmetric homoditopic receptor,[1] which is based on a binaphthyl chiral skeleton with 2,2´-diisopropoxy substituents and a common binding side arm, (o carboxamido)-trifluoroacetophenone,[2] in the 3,3´-positions, which recognizes α-amino acids as their amino carboxylate forms through formation of stabilized adducts, has been synthesised. Very high enantioselectivities ranging from 78:22 to 96:4 (L-AA: D-AA) for various racemic amino acids were achieved.References1) Park, H.; Kim, K.M.; Lee, A.; Ham, S.; Nam, W.; Chin, J. J. Am. Chem. Soc. 2007, 129, 1518.2) 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.



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Efficient Synthesis of Indolizine with Organoindium Reagent

이광무, 손익환, 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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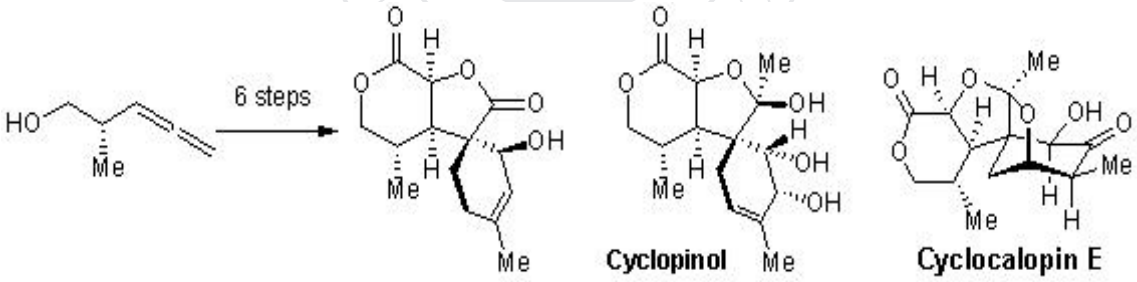
발표종류: 포스터, 발표일시: 목 10:30~12:30

Enantioselective Synthesis of Sylvone through Michael Addition

양대석, *유범선, 최지훈, *이민경, 유찬모

*성균관대 화학과 *성균관대 화학과 화학물질과학사업단*

Recently, we have developed a new method regarding allenoate adol process in high levels of enantioselectivity. In light of this result, we turned our attention for the synthesis of naturally occurung sylvone. 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) Micael addition of lithium dithiane to the a,b-unsaturated ester 2) Synthesis of sylvone. Stereoselectivity and mechanistic details will be presented.



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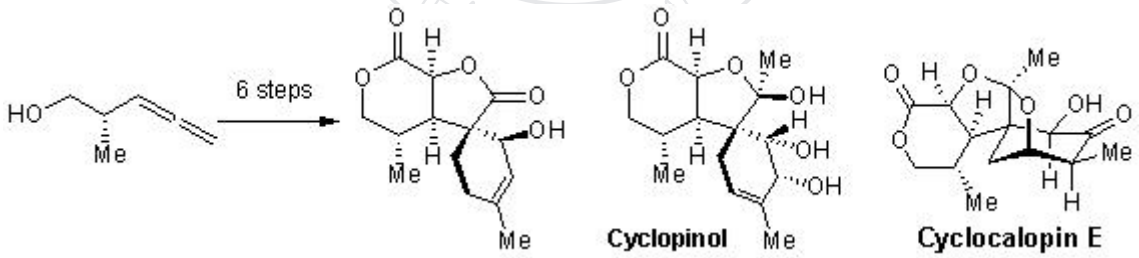
Directed Toward Synthesis of Cyclocalopin Series via New Cyclization Method

유범선, 이민경, 유찬모

성균관대 화학과 화학물질과학사업단

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Chemists are attempting to investigate some of these intricate pathways and develop methods to prepare similar products in the laboratory. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring cyclocalopin series: 1) elaboration of stereoselective construction of a spiro-unit of tricyclic core via a cycloaddition; 2) synthetic studies toward an enantioselective synthesis of cyclocalopin A.



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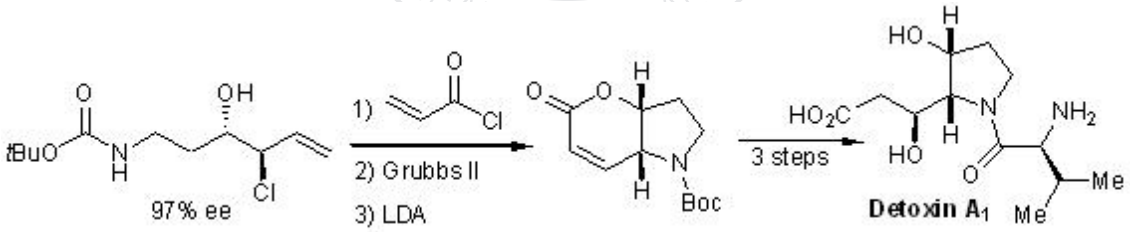
Stereoselective Chloroallylboration for the Synthesis of Chlorohydrins: Synthesis of Detoxine

성원제, 김다은, 김지희, 유찬모

성균관대 화학과

Development of stereo-controlled consecutive processes can offer advantages over stepwise transformations by increasing chemical efficiency and saving effort due to a simple operation. Recently, we developed a new synthetic method for the synthesis of all 4 possible chlorohydrins stereoselectively. We would like to present herein several crucial points that have emerged from our recent investigations: 1) Construction of bicyclic system starting from the chlorohydrin. 2) enantio- and diastereoselective synthesis of Detoxin naturally occurring A.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of Dithienosilole Derivatives

강동진, *강영진, 이필호

*강원대 화학과 *강원대 과학교육과*

The conversion of solar energy is one of the important technologies that can replace fossil fuels in the generation of mass energy. However, the high cost of solar panels made from traditional inorganic semiconductors imposes a restriction on their mass usage. Dye-sensitized solar cells (DSSCs) is a relatively new class of low-cost solar cell. In despite of several disadvantages, DSSCs are currently undergoing rapid development to obtain robust, efficient, and cheap devices that are suitable for practical use. Recently, we have synthesized dithienosilole derivatives that contain triarylamine moiety for use in DSSCs. The electron-donating moieties are triarylamine, and the electron-withdrawing parts are cyanoacrylic acid group. The synthesis of these compounds was accomplished by Stile cross-coupling reaction of dithienosilole with triarylamine in good yields.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

Amino acid, Methionine based turn on chemical sesnor for Hg(II) in aqueous solution

양미화, Lohani Chuda Raj, 이건형

인하대 화학과

Dansyl labelled methionine was synthesized in solid phase synthesis. The sensor that have a simple structure shows highly sensitive and selective response only to Hg(II) ions among various heavy and transition metal ions. The sensor detected Hg(II) ions in water by turn on or turn off response depending on the solvent. In this work, we described the binding stoichiometry of the sensor play an important role in the response type to Hg(II) ions.

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Colorimetric and fluorescent sensing of pyrophosphate in 100% aqueous solution by a system comprised of rhodamine compound and Fe3+ complex

장수정, 이건형

인하대 화학과

We developed a simple dual signal (color and “Off-On” fluorescent change) ensemble system based on the complex between a rhodamine compound and Fe3+ for the detection of pyrophosphate in 100% aqueous solutions. The complex between the rhodamine compound and Fe3+ was utilized as a chemosensing ensemble for the first time. The ensemble showed highly sensitive and selective fluorescent and colorimetric response to PPi among the anions in 100% aqueous solutions and no interference of the potent biological competitors including ATP, ADP, and phosphate for detection of PPi in 100% aqueous solutions at pH 7.0.

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Exceptional enantioselective transesterification of amino alcohols by Candida rugosa lipase

민보라, *심용균, **박지민, **박성순, ***이혁

*성균관대 화학과 *연세대 화학과 **성신여대 화학과 ***한국화학연구원 신약연구단*

Enzymatic kinetic resolution of racemic alcohols via acylation or hydrolysis has been broadly studied as one of the most effective methods for the preparation of optically active alcohols. Amino alcohol moieties with a certain stereochemistry infer interesting biological activities to organic compouds. Lipase-catalyzed enantiomeric kinetic resolution of amino alcohols was performed. N-Boc protected 4-aminobutan-2-ol (1) was synthesized, and several kinds of lipases were screened for the transesterification of this substrate. Several lipases showed high activities and enantioselectivities to afford the corresponding enantioselective ester (2) of (R)-4-aminobutan-2-ol. On the other hand, Candida rugosa lipase (CRL) favored the (S)-enantiomer. To examine this phenomenon, We used a combination of molecular modeling of lipase-transition state analogue complexes and kinetic measurements to identify the molecular. The computational modeling of transition state analogues bound to CRL shows that hydrogen bond between carbamate moiety in N-Boc protected 4-aminobutan-2-ol and ser450 in CRL This hydrogen bond may account for the reversal of enantioselectvity. Several amino alcohols were prepared and tested for the kinetic resolution by transesterification using CRL, and, as expected, the (S)-enantiomers of those derivatives were selectively acylated by CRL.

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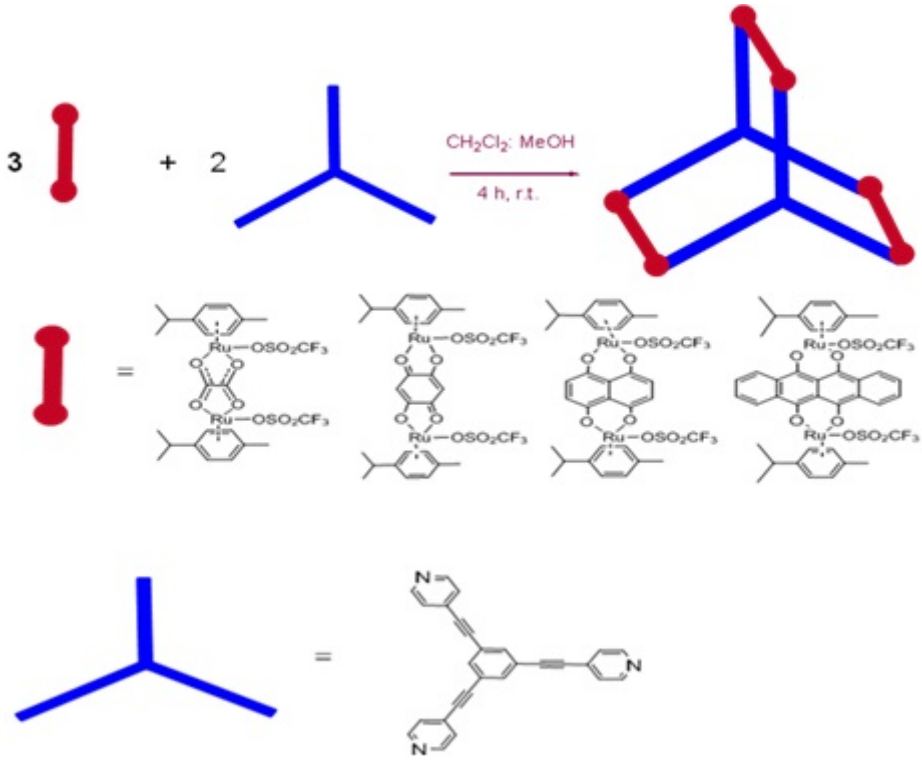
Self-Assembly of Nanoscopic Ruthenium Prismatic Cages and Their Anticancer Activity

vajpayee vaishali, 송영호, 최영화, 지기환

울산대 화학과

Metallo-pharmaceuticals are playing a significant role in therapeutic and diagnostic medicine; the discovery and development of new metallo-drugs remain an ever-growing area of research in medicinal inorganic chemistry. Our research objective is the design and application of self-assembled supramolecules, which motivated us to explore the potential of ruthenium prismatic cages as metallo-pharmaceuticals. Various ruthenium prismatic nano-cages were arranged by molecular programmed self-assembly of ruthenium clips and tridentate organic donor, and characterized by NMR, ESI-MS and X-ray crystallography. One of the main challenges in cancer chemotherapy is to develop drugs that are selective towards cancer cells in order to reduce the general toxicity and consequently the side effects of the compound. One such targeting method involves using large carrier compounds which release the drug once inside a cancer cell, since large compounds selectively accumulate in cancer cells owing to their enhanced permeability and retention effect. Herein, specific ruthenium nanocage represents the carrier compound and its high charge also potentially facilitates uptake in cancer cells. In particular, this supramolecule inhibits proliferation of SK-hep-1, HeLa, A549, MDA-MB-231, and HCT 15 cells in culture at low micro-molar concentrations, which is found to be considerably stronger than the inhibitory concentration of the benchmark drug, Cisplatin.



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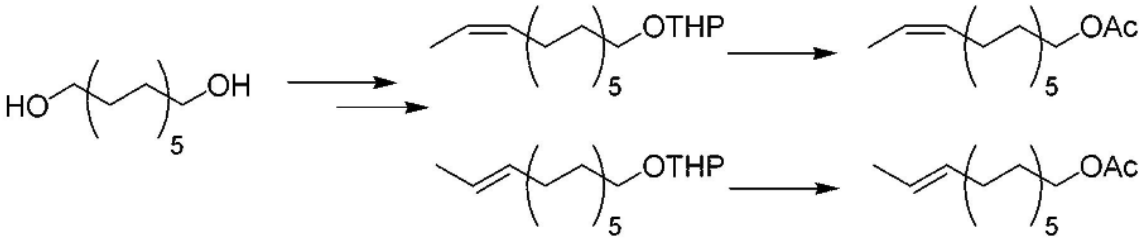
New Synthesis for Sex Pheromones of the Asian Corn Borer Moth

김인숙, *홍용표

*(주)그린아그로텍 부설연구소 *안동대 응용화학과*

Sex pheromones of the asian corn borer moth, (Z)-12-tetradecen-1-yl acetate and (E)-12-tetradecen-1-yl acetate were synthesized from 1,12-dodecanediol. 1,12-dodecanediol was monoprotected by DHP and oxidated to aldehyde. Dodecanal THP ether and ethyl triphenylphosphonium bromide gave stereoselectively *cis*- product by Wittig reaction. On the other hand, *trans*- product was prepared by schlösser modification.



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Efficient Carbon-Sulfur Cross-Coupling Reactions

엄다한, 이필호

강원대 화학과

The sulfide group is a key motif in chemistry and biology. Because of the characteristic features of C-S bond as functions of biological, pharmaceutical, and material sciences, transition metal, such as Pd, Ni, Cu, Co, Rh, and Pt catalyzed C-S bond formations have received much attentions and grown up by means of the development of new catalytic systems and appropriate reagents. Recently, we reported novel and efficient Pd-catalyzed C-C cross-coupling reactions using allylindiums, allenylindiums, tri(organo)indiums, and tetra(organo)indates on the basis of the intriguing chemical properties of indium metal. However, C-S cross-coupling reactions using organoindium reagents have not been reported despite one of the principal methods forming C-heteroatom bonds. These results have led us to investigate the participation of organoindium reagents in C-S cross-coupling reactions. We report that indium tri(organothiolate) are effective nucleophilic coupling partners in Pd-catalyzed C-S cross-coupling reactions with a variety of electrophiles to produce functionalized sulfides in excellent yields with high atom efficiency and complete regio- and chemoselectivity. Also, we prepared indium tri(allyl thiolate) compound using allyl thiol and indium.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of Recyclable Photosensitizers and Photochemical Fabrication of Silver Nanostructures at the Solid–Liquid Interface Using a Recyclable Reduction Process

김성식, *M. Sakamoto, *M. Fujitsuka, *T. Majima

*전북대 화학과 *Osaka University*

Photochemical synthesis of metal nanostructures through photosensitized reduction of metal sources is a powerful method in a wide variety of environments, because light can selectively promote the desired reaction without damaging the surrounding environment. A drawback of the method is that most organic photosensitizers are disposable and consumed during the photochemical reactions and as a consequence a much larger amount of photosensitizer than that of the metal source is usually required, and therefore, the photosensitized reduction method is wasteful in terms of the sensitizer. In the present work, we propose a new photochemical synthetic method using a recyclable photosensitizer and applied it to fabricate Ag nanostructures at the solid–liquid interface. The photosensitized reduction of Ag ion at the solid–liquid interface resulted in the formation of unique Ag nanostructures (nanowires or plates) without the use of templates or stabilizing agents. The relation between the morphology and several externalcontributing factors, such as solvent polarity and interaction between the substrate and crystal phase, was discussed.

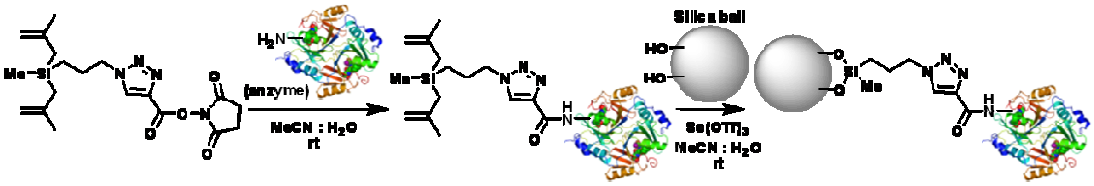
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-236**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile immobilization of enzyme onto solid support through chemical modification of enzyme by NHS-ester functionalized methallylsilane

이세라, 전철호

연세대 화학과

In this report, the efficient immobilization of enzyme onto solid support through direct chemical modification of enzyme is presented. In our method, free enzyme was treated with methallylsilane containing NHS-ester group, which is reactive for primary amine group of lysine residue on enzyme. Then, the resulting modified enzyme was immobilized onto solid support such as silica ball and glass by $Sc(OTf)_3$ catalyst. As a model enzyme, glucose oxidase or lipase was used, and the immobilization rate of enzyme was determined by activity test of these enzymes on solid support. It was found that the immobilized enzyme prepared by this protocol with chemically modified enzyme showed a higher activity than one prepared by conventional grafting immobilization method.



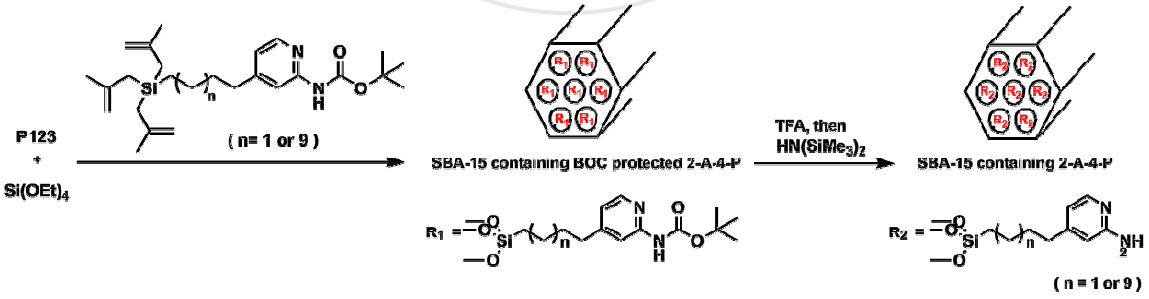
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-237**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of Functional Group-immobilized Mesoporous Materials using Methallylsilane Derivatives

지혜정, 전철호

연세대 화학과

A new synthetic method for fabrication of SBA-15 using methallylsilane derivatives is presented. Methallylsilane is chosen as a co-condensation partner due to stability and lability in acid condition suitable for preparing SBA-15. The co-condensation reaction of TEOS and functionalized methallylsilane in the presence of P123 was carried out to afford SBA-15 bearing functional group such as azido group. Especially, using 2-amino-4-picoline, known as a chelation-auxiliary organic catalyst, 2-amino-4-pyridinyl group-immobilized SBA-15 was prepared by this method. The resulting material was used for the immobilized catalyst hydroacylation.



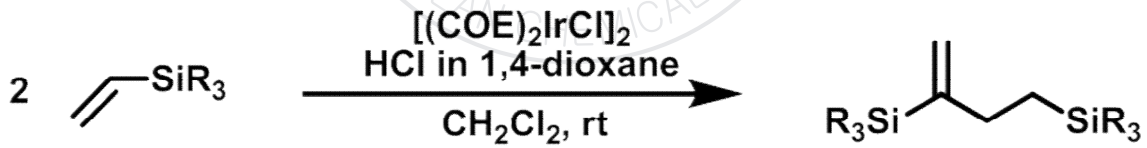
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-238**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Efficient Dimerization of Vinyilsilane by $[(COE)_2IrCl]_2$ and HCl Catalysts

박성준, 박정우, 최지환, 전철호

연세대 화학과

In this report, efficient catalytic system consisting of $[(COE)_2IrCl]_2$ and HCl catalysts for dimerization of vinylsilane is presented. The reaction is thought to proceed by metal-hydride insertion of in-situ generated iridium(III) hydride to vinylsilane and consecutive carbometallation of iridium-ethylsilyl complex, followed by beta-hydride elimination of the resulting carbometallated dimeric silyl complexs. This reaction proceeds regioselectively under very mild condition to afford meso-type dimer. The synthetic scope of this vinylsilane dimerization is also presented.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-239**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Meerwein-Ponndorf-Verley Reduction with Indium Isopropoxide

이재영, 이필호

강원대 화학과

Among the various methods for reducing carbonyl groups, the Meerwein-Ponndorf-Verley (MPV) reduction is a long-established and still important method in organic synthesis. The MPV reduction of ketones and aldehydes uses inexpensive and environmentally friendly iPrOH as a hydride source and aluminum alkoxides as catalysts. However, aluminum-mediated MPV reduction is limited by its requirement of a stoichiometric amount of the aluminum alkoxide catalyst and sometimes low yields due to side reactions. Recently, we report the MPV reduction of aldehydes using indium reagent.

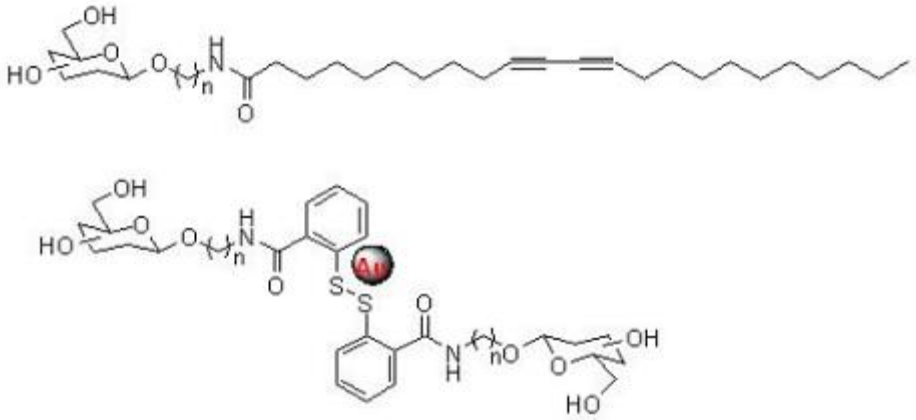
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-240**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Functionalization of Anomeric Center in Carbohydrate Derivatives: Application to Bio-Sensor Technologies

최진선, 장은희, 김미형, 안철진

창원대 화학과

Carborhydrates 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 carbohydate 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.



[n=2, 6, 10]

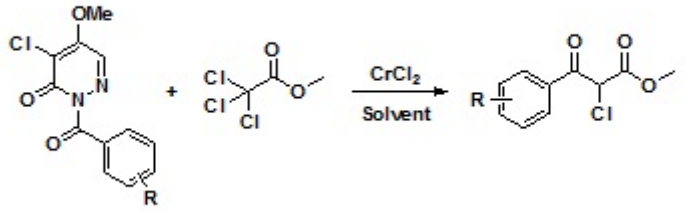
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-241**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

CrCl2-mediated condensation of pyridazione derivatives with methyl trichloroacetate

최경민, *윤용진, 신동수

*창원대 화학과 *경상대 화학과*

Methyl 2-chloro-3-oxo-3-phenylpropanoates were prepared by the reaction of pyridazione derivatives with methyl 1,1,1-trichloro acetate using CrCl2-mediated condensation. The more detailed reaction methodology will be discussed.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-242**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

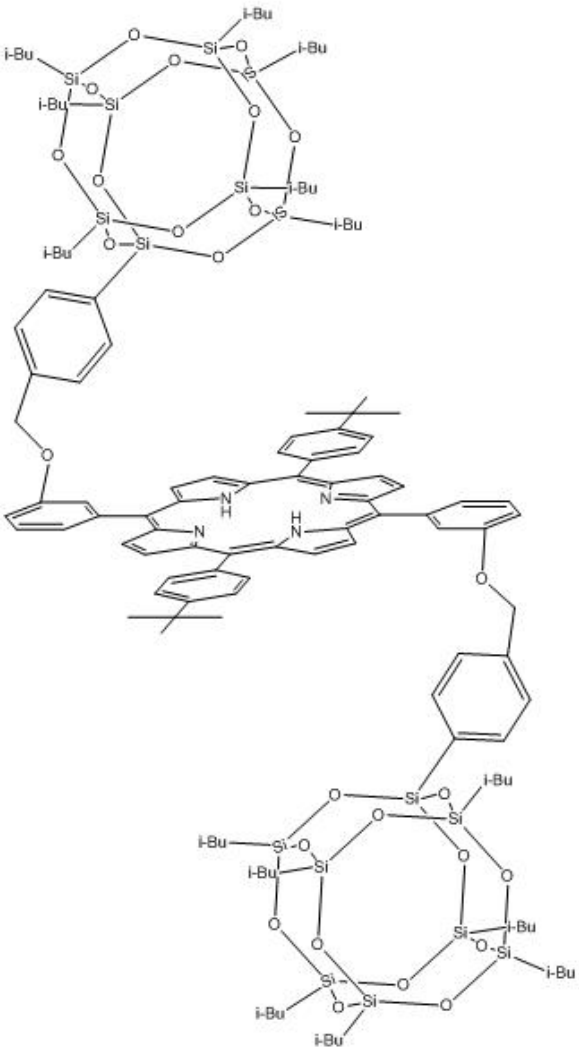
Effects of Polyhedral Oligomeric Silsesquioxanes (POSS) on Anion Detection of Porphyrin Chemosensors

정은희, *장진영, *전새롬, **이창희

*강릉대 화학과 *강릉대 화학신소재 **강원대 화학과*

We have synthesized the series of porphyrins which incorporating polyhedral oligomeric silsesquioxanes (POSS) units. Studies on their spectroscopic properties and chemical sensing abilities which depends on the numbers of POSS units and the relative position of POSS at the porphyrin sensors have performed. It would lead to the development of new colorimetric chemosensors which are more convenient, specific and sensitive than the previously developed porphyrin sensors.

THE KOREAN CHEMICAL SOCIETY



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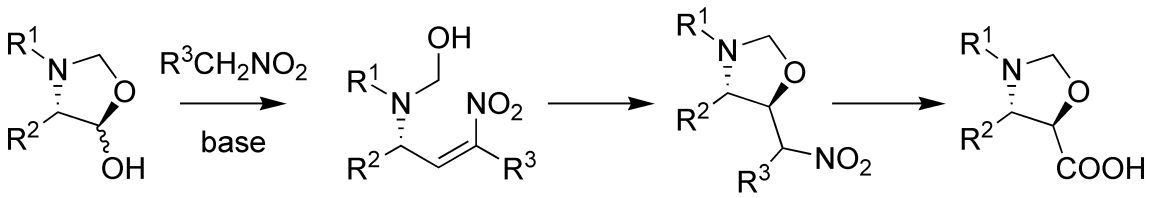
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-243**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Study for an efficient synthesis of β–amino-α-hydroxy acids

서영란, 김현정, 김영규

서울대 화학생물공학부

We have reported the preparation of some biologically active γ-amino-β-hydroxy acids such as (-)-statin and threo-β-hydroxyglutamic acid by the stereoselective intramolecular conjugate addition of an N-hydroxymethyl group onto γ-amino-α,β-unsaturated esters. As an extension of the method, a synthetic study for biologically and pharmaceutically important β–amino-α-hydroxy acids is presented here. As in the scheme shown below, the precursors to β–amino-α-hydroxy acids are first obtained by the stereoselective conjugate addition of the N-hydroxymethyl group onto the nitroolefin, and then functional group conversions of the precursors with a nitro group result in the desired target compounds. Thus, the nitro group is used here as a carboxylic acid equivalent as well as a Michael acceptor in the intramolecular conjugate addition.



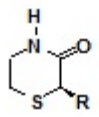
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-244**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of (Z)-2-alkylidene-4-(1-phenylethyl)-3,4-dihydro-2H-benzo[b][1,4]thiazine-3(4H)-thiones

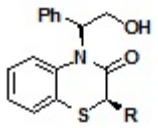
이은영, 이상길, 김신형, 원태진, 신동수

창원대 화학과

2-Substituted thiomorpholin-3-one (2-STMO) 1 is a pharmacophore of great interest and derivatives containing such a sub-unit have already been prepared and evaluated in various biological fields. As one part of preparing [1,4]thiazine-3-thione scaffold, 2- substituted (R)-4-(2-hydroxy-1-phenylethyl)-2H-benzo[b][1,4]thiazin-3(4H)-one 2 were prepared by the reaction of (R)-4-(2-hydroxy-1-phenylethyl)-2H-benzo[b][1,4]thiazin-3(4H)-one via Smiles rearrangement using microwave irradiation by one-pot synthesis, followed by the reaction with alkyl halide in LDA base.



1



2

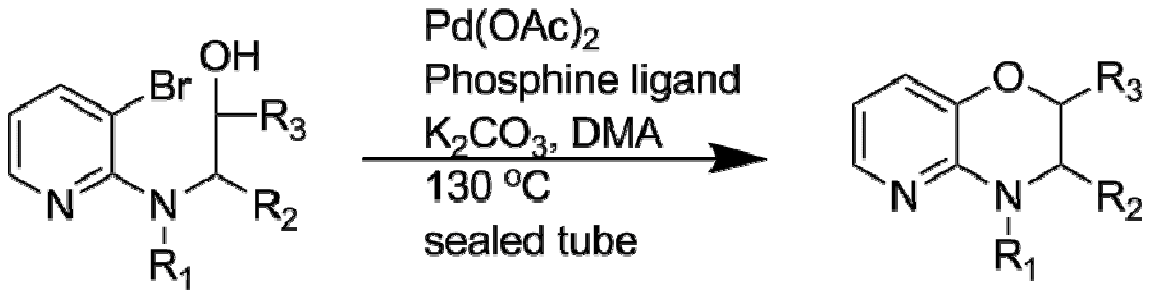
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-245**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Pyrido[3,2-*b*][1,4]oxazines via Palladium-catalyzed Intramolecular Cyclization of Aminonoalcohol-tethered 3-bromopyridines

김정근, *최지원, **양은혜, 하덕찬, **하재두

*고려대 화학과 *서강대 화학과 **한국화학연구원 난치성질환치료제연구센터*

3,4-Dihydro-2*H*-pyrido[3,2-*b*][1,4]oxazines often display important biological activities. Although several methods for the synthesis of various 3,4-Dihydro-2*H*-pyrido[3,2-*b*][1,4]oxazines have been described in the literature, those methods suffered in terms of low yields and were hard to give the optically pure compounds. Key intermediates, 2-(3-bromopyridine-2-ylamino)alcohols were obtained through a rapid nucleophilic substitution reaction of 3-bromo-2-chloropyridine with various aminoalcohols under microwave irradiation. With 2-(3-bromopyridine-2-ylamino)alcohols in our hands, palladium-catalyzed cyclization reaction of 3-bromoaminoalcohols cleanly afforded the pyrido[1,4]oxazine derivatives in 50-80% yield. Using this method, we can readily obtain optically pure 3,4-dihydro-2*H*-pyrido[3,2-*b*][1,4]oxazines with various substituents.



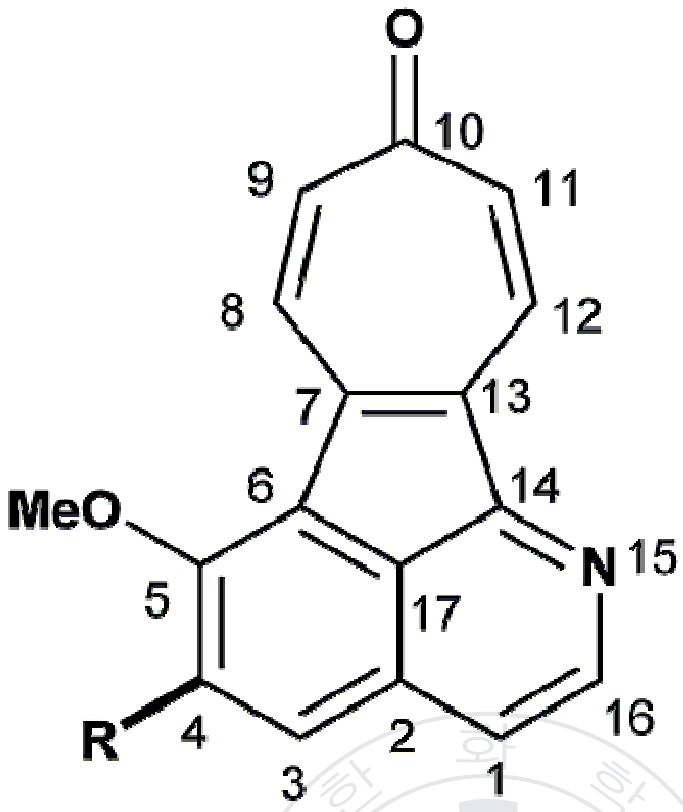
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-246**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthetic Study of 4-Demethoxypareitropone

신나라, 김현정, 김영규

서울대 화학생물공학부

Pareitropone, the most effective tropoloisoquinoline alkaloid against the leukemia P388 cell line (IC50 = 2.7 nM), is an attractive synthetic target because of its unique structural architecture and potent cytotoxicity. Since our total synthesis of pareitropone (1), we have been working on total syntheses of pareitropone analogues to study the structure-activity relationship. A synthetic study of one of the analogues without a methoxy group at C-4, 4-demethoxypareitropone (2), is reported here. Applying the synthetic protocol developed for the total synthesis of pareitropone, the target compound 2 is to be prepared from o-vanillin mainly via a Suzuki aryl-aryl coupling, a Pomeranz-Fritsch isoquinoline formation, a Reissert-type nitromethylation on the resulting isoquinoline ring and a Kende radical anion coupling of the phenolic nitronate.



R = OMe: Pareitropone (1)
R = H : 4-Demethoxypareitropone (2)

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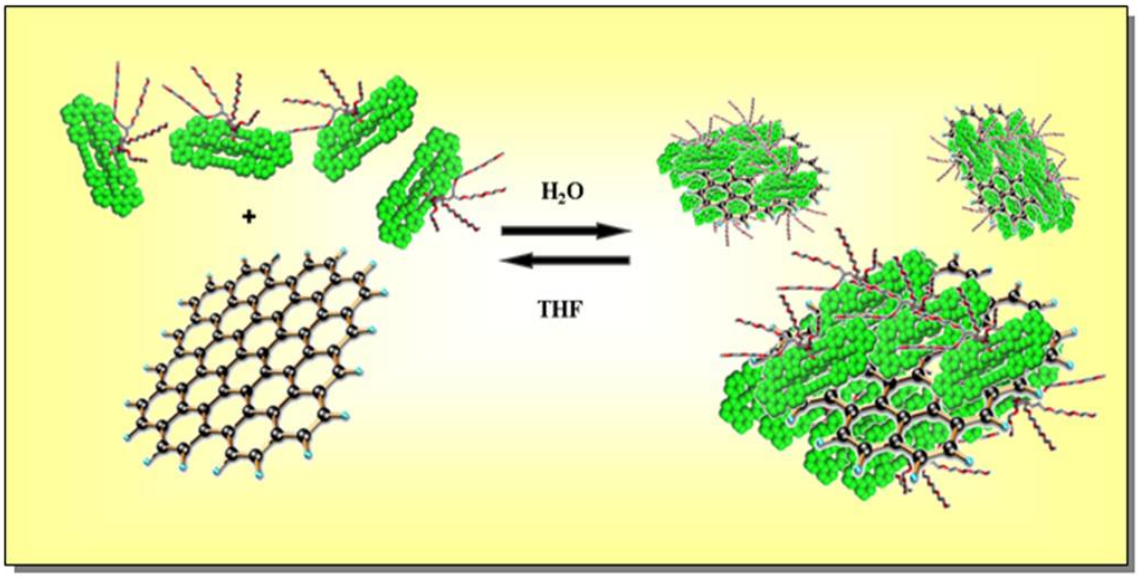
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-247**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Self-Assembly of Amphiphilic Disks

김태훈, *이명수

*서울대 화학부 *서울대 화학과*

We have synthesized amphiphilic macrocycles with a planar thumbtack-like aromatic segment containing oligoether dendrons. These amphiphlic macrocycles can self-assemble into micelles, fibers and vesicles depending on their molecular sizes and shapes. The most notable feature of the thumbtack-like macrocycles investigated here is their ability to exfoliate graphene by pi-pi interaction in water. Such graphene exfoliation with these macrocycles may provide a new strategy for a more efficient way to get a high quality graphene and a good application of electrical substrates.



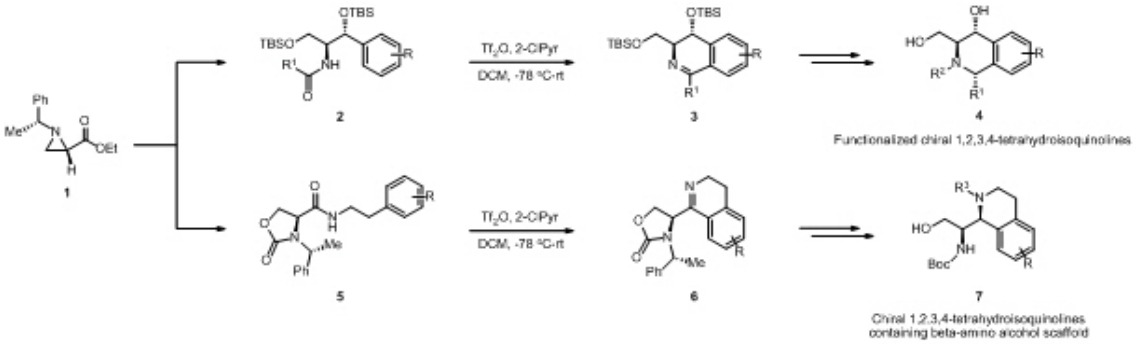
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-248**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Elaboration of Chiral Aziridine-2-carboxylate; Asymmetric Synthesis of 1,2,3,4-tetrahydroisoquinolines

김종찬, 강경연, 이규명, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

Substituted tetrahydroisoquinolines can be found in many pharmaceutically important molecules and attract interests from chemists due to their biological activities. Therefore, we were interested in the synthesis of enantiomerically pure 1,2,3,4-tetrahydroisoquinolines starting from chiral aziridines. Functionalized chiral 1,2,3,4-tetrahydroisoquinoline alkaloids 4 are synthesized from chiral (3,4-dimethoxyphenylethyl)amide initiators 2 derived from (S)-ethyl 1-((R)-1-phenylethyl)aziridine-2-carboxylate 1 via modified Bischler-Napieralski cyclization and stereoselective reduction of the corresponding imine products 3 in high yield. Also, the synthesis of chiral 1,2,3,4-tetrahydroisoquinolines containing ′ -amino alcohol scaffold 6 is successfully achieved via Bischler-Napieralski cyclization from an oxazolidine-4-carboxamide 5. Various substituents are attached to the nitrogen of 1,2,3,4-tetrahydroisoquinoline after stereoselective reduction of the imine.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-249**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Pd-Catalyzed Cross-Coupling Reactions of Aryl Halides with Vinyl Propagyl Bromide and Indium

김상혁, 박상준, 이필호

강원대 화학과

Enynes have been receiving considerable attention in organic synthesis. The famous antibiotics such as calicheamicine and dynemicin have conjugated enyne moiety as the essential structure for their biological activities. Enynes are also very important compounds in synthetic organic chemistry. Enynes are fundamental building blocks in organic synthesis. The synthesis of enynes has received special attention in these days and some methods have already been published. However, the synthetic method of cross-coupling reactions of aryl halides with functionalized propagyl bromide is still rare in organic reactions. So, we are interested in the synthesis of enynes and have developed method of Pd-catalyzed cross-coupling reactions of aryl halides with indium reagent.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-250**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Characterization of Poly(fluorene) Derivatives Containing Silole

박현태, 강소희, *장재완, 김윤희, **권순기

*경상대 화학과 *경상대 고분자공학과 **경상대 나노신소재공학부*

The design of new emissive and charge transport molecular materials has resulted in high performance OLEDs that are approaching the standards required for display applications. However, new materials and device architectures aimed for further improvements in device efficiency, lifetime and operating voltage are continuously being sought in different laboratories worldwide. High device efficiency and low operating voltage are particularly desirable for high performance OLEDs in display and solidstate lighting applications. Recently, silole or silacyclopentadiene derivatives have been proposed as a new class of electron transporting and highly fluorescent materials that can be used in their neat forms in OLEDs. Silole is a silicon-substituted cyclopentadiene with strong electron-accepting properties. The large electron affinity (and therefore low-lying lowest unoccupied molecular orbitals (LUMO)) is attributed to the σ*-π*conjugation between the σ* orbital of the two exocyclic Si–C σ-bonds and the π* orbital of the butadiene moiety on the silole ring. This interaction results in lowering the position of the LUMO level and suggests that siloles have the potential to serve as good electron transport materials.In the present study, we designed new polyfluorene derivatives containing silole. We will discuss the physical properties and device characteristics of new developed polymers.

일시: 2010년 10월 14~15일(목~금) 2일간
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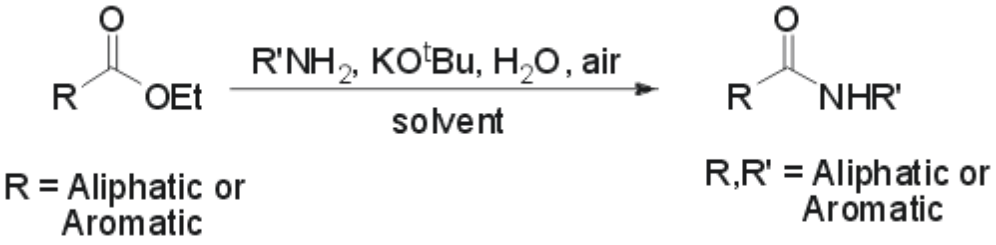
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

tert-Butoxide-assisted Amidation of esters

이인혜, 김보람, 김은정, *김점종, 윤용진

*경상대 화학과 *한국전자통신연구원 차세대태양광연구부*

Amidation is the most fundamental and important process in the organic synthesis. Amidation of the reactive carboxylic acid derivatives such as acyl halide, anhydride, and carboxylic acids is relatively easy. Amidation of the esters, however, is difficult under mild condition except for catalytic conditions due to their low reactivity. We investigated on *tert*-butoxide-assisted reaction of esters. Herein, we present mild and rapid amidation of esters with amines in the presence of KO^tBu and water in air.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

Intramolecular Cyclization Catalyzed by Iron

신두섭, 서석진, 이필호, *김성각

*강원대 화학과 *KAIST 화학과*

Development of an efficient cyclization method is very important for the biological and pharmaceutical applications. Fe-catalyed hydroarylation of arene-alkynes has attracted much attention in the pivotal areas of synthesis of conjugated aromatic compound in an atom-economical manner. Moreover, the importance of its intramolecuar reaction has been widely recognized as a feasible approach to cyclic vinylarene frameworks. Fe-catalyst for the electron-donating group substituted arene-alkynes, showed as high efficiency catalyst.

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발표코드: **ORGN.P-253**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

New fluorescent and electrochemical sensors for Hg(II)/anions based on pyrene appended ferrocene unit

CAO QIANYONG, 김종승

고려대 화학과

New mono- or bi- pyrene appended ferrocenes have been synthesized, and their fluorescent and electrochemical sensing toward various metal ions and anions were investigated. These compounds showed a pronounced multi-response toward metal ion Hg^{2+} and some anions such as F^-, $H_2PO_4^-$, PPi, with fluorescence change (increase or decrease), and the ferrocene/ferrocenium potential a large shift. Their binding mechanism is also discussed.

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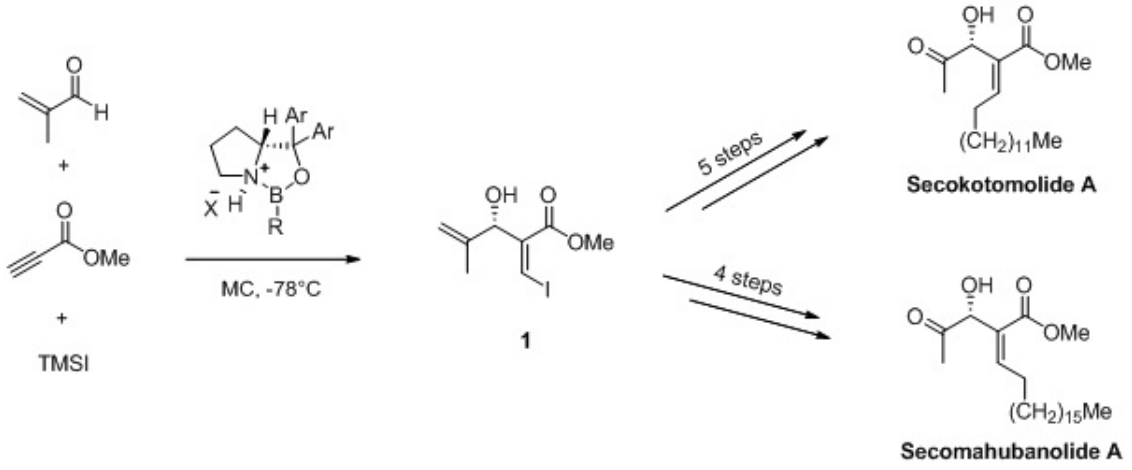
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Total Synthesis of Secokotomolide A and Secomahubanolide A

문순영, 이성일, 류도현

성균관대 화학과

Secokotomolide A and Secomahubanolide A were isolated from cinnamoum ketones and machilus zuihoensis respectively. Secokotomolide A was found to induce significant cell death in the human HeLa cell line by apoptotic-realted DNA damage. Secomahubanolide A shows marginal cytotoxicity against NUGC and HONE-1 cancer cell lines.The enantioselective synthesis of Secokotomolide A and Secomahubanolide A, has been accomplished from the readily available chiral (Z)-′ -iodo Morita-Baylis-Hillman ester (1) as a key intermediate. Asymmetric three component coupling reaction furnished (Z)-′ -iodo MBH ester (1) in high enantioselectivity. Additional few steps afforded both natural products in high overall yield.



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장소: 대구엑스코
발표코드: **ORGN.P-255**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Preparation of conductive polymer films from vapor phase polymerizable heterocyclic monomers

김병관, *김정훈, *김은경

*연세대 화공생명공학과 *연세대 화학공학과*

The vapor phase polymerizable monomers were newly synthesized for highly conductive polymer films. The iron(III) p-toluenesulfonate was used as an oxidant for polymerization and conveniently coated on various substrates. The vapor phase polymerization (VPP) was carried in a monomer filled chamber to result conductive thin film deposit on various substrates including paper, glass, and plastic films. In particular, the conductive polymer film coated on a flexible substrate showed good bending properties with high electrical conductivity. Herein we report the synthetic methods of monomers and the electrical properties of the resultant conductive polymers.

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발표분야: 유기화학
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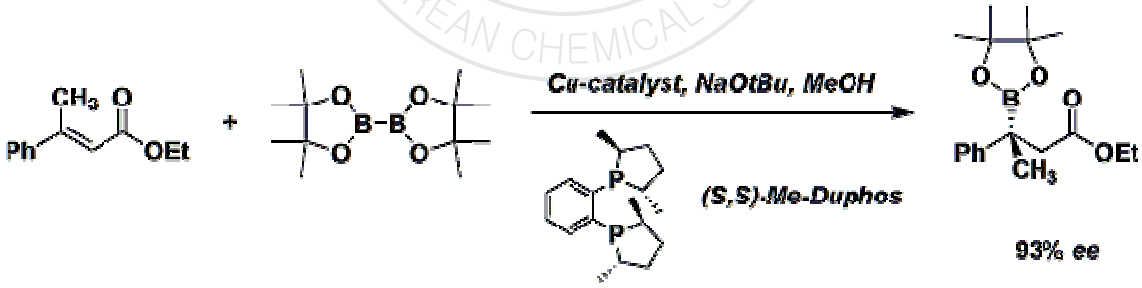
Copper-Catalyzed Enantioselective Boron Addition to β, β-disubstituted Conjugate Esters

풍신혜, 윤수경, 윤재숙

성균관대 화학과

In recent years, the transition-metal-catalyzed addition of diboron reagents to α, β-unsaturated carbonyl compounds, like acylic esters, ketones, amides and cyclic ketones, which afford organoboronate products with carbonyl functionalities at the β-position, has been widely investigated. Herein, we have developed a catalytic enantiselective conjugate boration system for acyclic β, β-disubstituted α, β-unsatutated esters to afford chiral tertiary organoboronic esters. Our chiral tertiary organoboron reagents can be utilized as a carbon nucleophile to form all carbon quaternary centers.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ORGN.P-257**
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발표종류: 포스터, 발표일시: 금 15:00~17:00

Efficient Preparation of Cyclohexenylmethyl Alcohols Possessing exo-Methylene Moiety

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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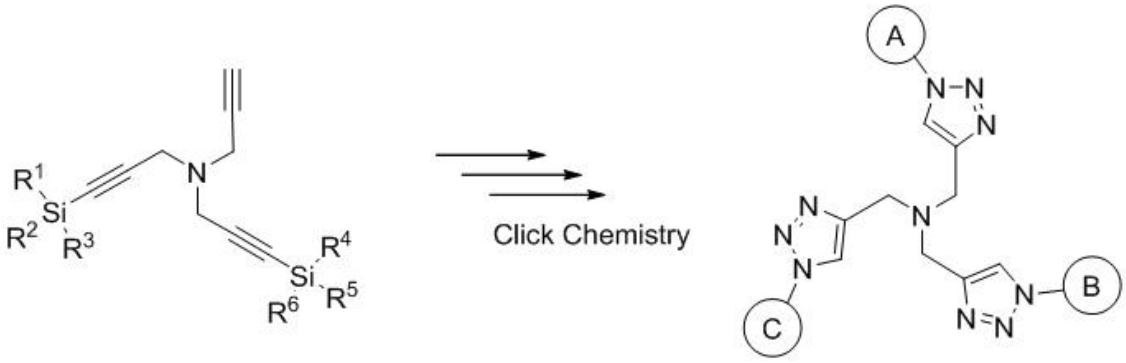
발표종류: 포스터, 발표일시: 금 15:00~17:00

Facile method for the conjugation of three diffent molecules

신동석, *김형백, **이병세, 지대윤

*서강대 화학과 *서강대 **(주)퓨처켐 표지화학연구소*

Tripropargyl amines with two different silyl protected groups have been synthesized for the use of multifunctional linker. Selective deprotection of silyl group followed by copper catalyzed alkyne/azide cycloaddition was recognized as a useful tool to prepare a tripodal linker, which could possess three different bioactive molecules. We demonstrated the preparation of silyl protected propargyl amines and a facile synthetic method of multifunctional compounds using successive click chemistry.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

Efficient micowave-assisted synthesis of 5-substituted thiazole derivatives with palladium catalyst

김지현, 염을균

충남대 화학과

Microwave irradiation afforded over conventional heating in chemical transformation, particularly the enormous acceleration of the reaction rate, significant energy savings, as well as high chemical yields and cleaner reactions. Recently, many microwave- assisted synthetic method were reported with palladium catalyst such as Suzuki, Stille, Heck reaction etc. Although thiazole derivatives are chemically and biologically interesting molecules due to their promising drug candidates and organic light emitting diode, but microwave-assisted palladium-catalyzed direct arylation of thiazole was not reported. In this research, we studied an efficient microwave-assisted direct heteroarylation with palladium catalyst of 5-substituted thiazole. The reactions were performed 5-substituted thiazole with heteroarylhalide under 5 mol% Pd(OAc)2, 1eq K2CO3 and NMP. The reaction provided high yield with short reaction time in 10 minutes.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Preparation of FMS-like tyrosine kinase-3 (FLT3) inhibitor

이도형, 이필호

강원대 화학과

The commercially available 2-amino-6-hydroxybenzothiazole was condensed with 2-bromo-4'-nitroacetophenone in refluxing ethanol to yield imidazo hydroxy benzothiazole ring attached directly to the p-nitrophenyl ring. This was reacted with N-chloroethylmorpholine to produce phenolic ether compound. Reduction of the nitro group using iron and HCl or stannous chloride gave the corresponding amines, which were coupled with 5-tert-butyl-isoxazole-3-isocyanate, to yield N-(5-tert-butyl-isoxazol-3-yl)-N'-{4-[7-(2-morpholin-4-yl-ethoxy)imidazo-[2,1-b][1,3]benzothiazol-2-yl]phenyl}urea. 5-tert-Butyl isoxazole-3-isocyanate was prepared from the commercially available 3-amino-5-tert-butyl-isoxazole by treatment with triphosgene.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Asymmetric Intermolecular Stetter Reaction of Acetaldehyde with Michael acceptors Catalyzed by N-Heterocyclic Carbenes

JINMINGYU, *김선민, 류도현, *양정운

*성균관대 화학과 *성균관대 에너지과학과*

The Stetter reaction is well-defined umpolung process in which NHC (N-heterocyclic carbene) have been successfully applied to build the 1,4-dicarbonyl compounds and related derivatives, such as 1,4-diketones, 1,4-ketoesters or 1,4-ketonitriles, which were depended on the Michael acceptors. Herein, we present the chiral NHC-catalyzed asymmetric Stetter reaction of a variety of Michael acceptors with acetaldehdye as biomimetic acyl anion source, affording the corresponding enantioenriched Stetter products in high yields with good enantioselectivities.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Cyclization of α-Alkynyl β-Ketoester Catalyzed by Iron

박영철, 이필호

강원대 화학과

The importance of cyclopentanoid natural products continuces inspire the development of methods for the synthesis of 5-membered rings. The intramolecular ene reaction of unsaturated ketones and aldehydes, namely, the Conia-ene reaction, is an important strategy; however, the high temperature needed severely limits its synthetic utility. The utility of this cyclization methodology has been significantly expanded in recent years by the use of metal catalysts, which has allowed the reaction to proceed at lower temperatures. Unfortunately, these transition-metal-catalyzed cyclizations are often needed additivies, such as strong base, strong acid, and photochemical activation. A catalytic version of the Conia-ene reaction that proceeds at ambient temperatures and under neutral conditions would dramatically increase the utility of this reaction. Herein, we report that iron catalyze the cyclization of ketoesters with alkynes to provide an effective synthetic method of 5-membered rings.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Recognition properties of 2-hydroxynaphthaldehyde containing Crown ethers and Quinoline

장승현, 최진욱

대구대 화학과

New luminescent crown ethers were synthesized. N-(4'-benzo-18-crown-6)-2-hydroxy-1-naphthaldehyde,3-((quinolin-8-ylimino)methyl)naphthalen-2-ol were prepared by reaction of 4'-aminobenzo-18-crown-6, 8-aminoquinoline and 2-hydroxy-1-naphthaldehyde. Binding interaction of the compound with metal cations was studied through absorption spectroscopy and emission spectroscopy.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Syntheses and Luminescent Characterization of N-(4'-benzo-15-crown-5)-2-hydroxy-1-naphthaldehyde

장승현, 최진욱

대구대 화학과

New luminescent crown ethers were synthesized. N-(4'-benzo-15-crown-5)-2-hydroxybenzaldehyde were prepared by reaction of 4'-aminobenzo-15-crown-5and 2-hydroxybenzaldehyde. N-(4'-benzo-15-crown-5)-2-hydroxy-1-naphthaldehyde were made by the reaction of 4'-aminobenzo-15-crown-5 and2-hydroxy-1-naphthaldehyde, respectively. Luminescence was increased by adding alkali metal ions. Luminescent15-crown-5 render fluroscence emission intensity responsive to added K+and, to a lesser extent, NH4+.

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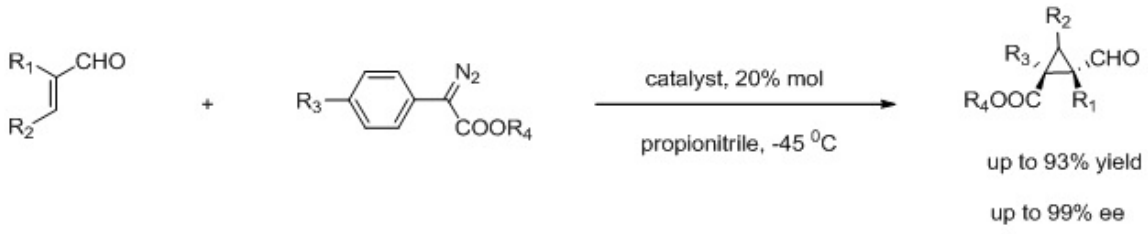
발표종류: 포스터, 발표일시: 금 15:00~17:00

Asymmetric cyclopropanation between aryldiazoacetates and substituted acroleins

gaolizhu, 류도현

성균관대 화학과

Cyclopropanation between diazocompounds and activated olefins have been extensively investigated and are presently well understood. However, there has been little work reported on asymmetric cyclopropanation with substituted acroleins. Catalytic synthetic approach to get the highly functionalized cyclopropane was investigated. In the presence of chiral oxazaborolidinium cation as a catalyst, asymmetric cyclopropanations provided various substituted cyclopropanes in high yield with high diastereoselectivity and enantioselectivity



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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Multifunctional Magnetic Nanoparticles for Targeted imaging and Therapy

록치충, 이영행, 채규윤

원광대 화학과

A simple and effective approach to the synthesis of multifunctional manganese-doped magnetism-engineered iron oxide (MnMEIO) nanoparticles was demonstrated and the effect of coupling agents and reaction time on controlling size of nanoparticles were studied. The morphology and uniformity of nanoparticles were investigated by XRD and TEM. Surface modification and composition were analyzed by FTIR and XPS, respectively. In addition, we demonstrated that the nanoparticles provide carboxyl functional group as a binding site for immobilization of targeting ligand in aqueous media.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Highly Positive Charged Calix[4]arene Derivatives: A molecular platform for siRNA delivery

박준원, 김종승

고려대 화학과

Calix[4]arene used as molecular platform to design various sensors, ion spore, MRI contrast agent and more recently DNA transfection materials. Currently in medical science it is very challenging to delivery of siRNA to cure deadly disease to the target cell. Generally cationic lipids are used as binding materials. As already reported that calix[4]arene derivatives have low cytotoxicity that encourage us to design calix[4]arene based cationic vehicle to deliver the siRNA to the cell. In connection with that we have synthesized calix[4]arene derivative in conjuction with tetra spermine unit at the lower rim of the calix[4]arene followed by four successive steps with high yield. In preliminary study we notice this new vehicle has good binding affinity with siRNA and transfection in vitro is underway.

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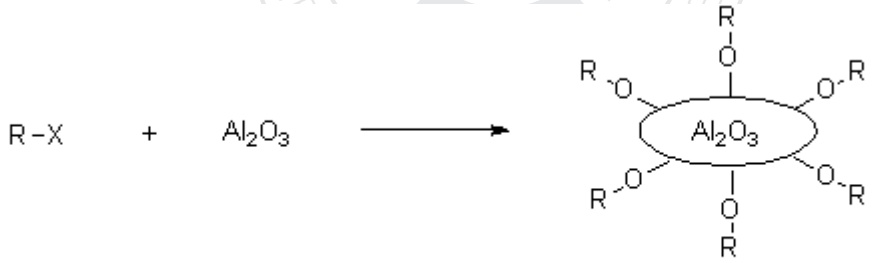
발표종류: 포스터, 발표일시: 금 15:00~17:00

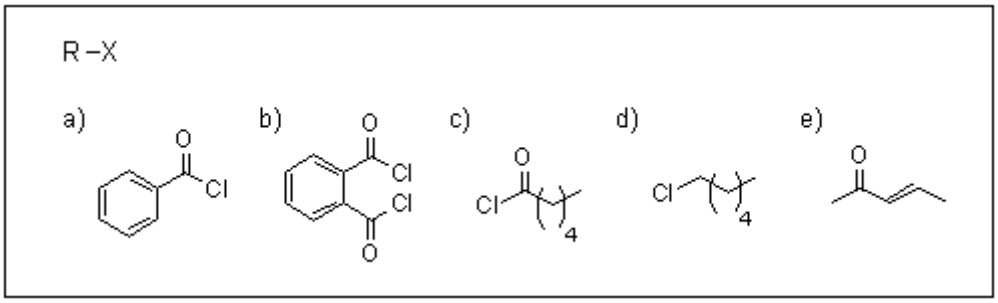
Functionalization of Porous-Alumina with Organic Ligands ; Luminescence Hybrid Material

장석명, 안철진

창원대 화학과

The functionalization of porous alumina with organic compounds is developed to prepare the organic-inorganic hybrid luminescent material. In this work 1]we will discuss the convinient reaction method which is microwave irradiation. 2]The characterization of organic-inorganic hybrid luminescent material will be discussed.





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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Ozonides from α-Terpinene and Terpinolene

이은희, 박형진, 구본석, 정인찬

한서대 화학과

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. At this time, when added carbonyl compounds outside, it synthesizes cross ozonide by inter cycloaddition between carbonyl oxide, so called reaction intermediate and carbonyl components be supplied outside. In this work, we have shown that ozone attacks the double bonds of conjugated 1,3-cyclodiene Ring(α-Terpinene) stepwise, in contrast to the reaction with nonconjugated cyclodienes. 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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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and characterization of acyl chitins

Lok Ranjan Bhatt, 남선미, 강경희, 채규윤

원광대 화학과

Acyl chitins were synthesized by the reaction of chitin with carboxylic acids in the presence of TFAA. The products were characterized by fourier transform infrared spectroscopy and scanning electron microscopy (SEM). The degree of O-acyl substitution for chitin derivatives was determined by FT-IR analysis. The solubility of the products was tested in various organic solvents. The products with the higher degree of acid substitution showed better solubility in various organic solvents. The results showed that TFAA promoted acylation of chitin with carboxylic acid is an easy and efficient method to prepare acyl chitins.

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A study on the efficient synthesis and characterization of acylated chitosans derivatives

안채영, *김보미, **김현, 채규윤

*원광대 화학과 *원광대 생명나노 화학과 **원광대 생명나노화학*

A series of acylated chitosan derivatives was prepared by reacting chitosan in a solution of TFAA and each of the hexyl, heptyl, octyl, decyl, lauryl and palmityl carboxylic acids. Prepared chitosan esters were characterized using FT-IR and 1H NMR. Their thermal property and morphology were analyzed using differential scanning calorimetry and scanning electron microscopy, respectively. The results showed that combining carboxylic acid(s) with chitosan provides a new copolymer(s) with improved physical properties including solubility.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of New Naphthoquinone Derivatives and Their antitumor activities in vitro

진선화, 정명훈, 권수한, 정용석

충북대 화학과

Quinones are widely distributed in nature and play essential biological roles. and some are used as anticancer drugs. In the study, new naphthoquinone derivatives were synthesized and the antitumor activities in HCT116 cell line were investigated.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Anthracene Organic Light Emitting Diodes and Evaluation of their physical properties

정명훈, 진선화, 권수한, 정용석

충북대 화학과

Blue light emission is very important for applying electroluminescent device to full display. As a candidate for emitting material of the blue OLED, new anthracene derivatives with a substituted naphthyl phenyl group were synthesized.We characterized the optical and electrical properties of the newly synthesized blue anthracene material.

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Highly selective and sensitive detection of Hg(II) in 100% neutral aqueous solution by dansyl labeled amino acids

Lohani Chuda Raj, 김정민, **Neupane Lok Nath**, 이건형

인하대 화학과

The recent development of selective and sensitive fluorescent tools capable of detecting heavy and transition metal ions has received attention due to prompt detection of small amounts of metal ions that have impact on human health and ecology. Mercury ions are a highly toxic heavy metal ion and, even very low concentrations of contamination caused a serious problem in environmental and health systems. Therefore, detection of Hg2+ ions in environment and living cells have been of great interest Here, we synthesized one or two dansyl labeled amino acids in solid phase synthesis and investigated detection ability to heavy and transition metal ions in 100% aqueous solution. Two dansyl labeled L-lysine residue among them shows only turn on response to Hg(II) in 100% aqueous solution. The sensor showed exclusive selectivity, high sensitivity (kd = 4.2 nM) and reversible monitoring. This sensor has satisfied for monitoring the maximum allowable level (2 ppb) of mercury ion in drinking water demanded by EPA. In addition, the sensor detected Hg2+ in live cells.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Design and synthesis of fluorescent dipeptide sensors and tuning metal selectivity of the peptides by amino acid variations

Neupane Lok Nath, 이건형

인하대 화학과

The detection and quantification of heavy metal ions are important in many applications, including environmental monitoring, waste management, developmental biology, and clinical toxicology. Recently, peptides sensors are frequently used to detect the heavy metal ions. Here, we synthesized three dansyl labeled dipeptides (Dan-Met-His, Dan-Met-Cys and Dan-Met-Trp) to analyze the selectivity of different metal ions in 100 % aqueous solution. The sensitivity, detection limit, stoichiometry, binding mode and reversibility of selective metal ions were also studied to their respective peptides.

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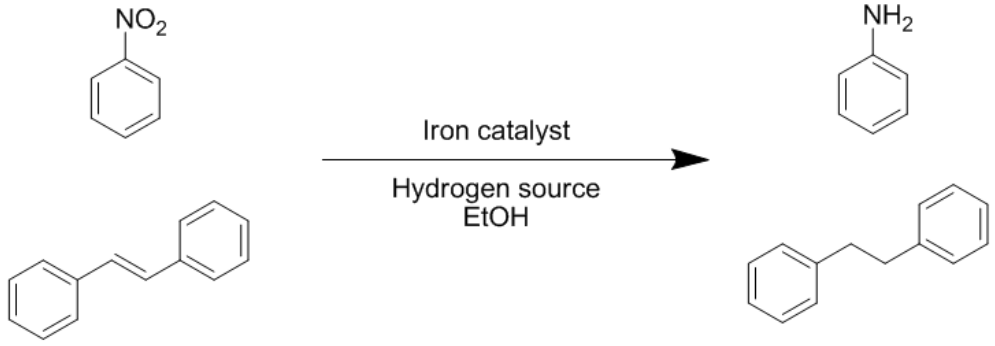
발표종류: 포스터, 발표일시: 금 15:00~17:00

Magnetically Recyclable Iron Oxide Catalyst for Selective Reductions

김세영, 정주영, *현택환, 김병문

*서울대 화학부 *서울대 화학생물공학부*

Recently, Iron(II) or (III) catalysts have attracted much attention due to their broad spectrum of applications such as cross-coupling, hydrogenation, reduction, oxidation, and cycloaddition reactions. However, most of the reported iron catalysts were homogeneous metal salts such as $FeCl_3$, $Fe(CO)_5$, and $Fe(acac)_2$. Therefore, the development of efficient and economically viable iron-mediated reaction conditions awaits further development and for this we focused on the heterogenization of iron catalyst and their application to hydrogenation and reductions. We have utilized rhodium-Fe_3O_4 bimetallic nanoparticles, nanosized Fe_3O_4 and commercially available Fe_3O_4 nanoparticles (



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Polymer-Supported Pentaethylene Glycol as a Facile Heterogeneous Catalyst for Nucleophilic Fluorination

JADHAV VINOD HANMANT, *장승호, **김동욱

*전북대 핵의학과 *전북대 의과대학 핵의학과 **전북대 의학과*

Polymer-supported pentaethylene glycols (PSpentaEG) as promising catalysts for nucleophilic fluorination with alkali metal fluoride (MF) could significantly enhance the nucleophilicity of MF and provide simple purification and recycling in the reaction. Furthermore, by their synergistic effect, the combination of PSpentaEG and a tert-alcohol media system showed tremendous efficiency in the fluorination of basesensitive substrates such as sec-alkyl halide.

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Study of Aggregation–Induced Emission Enhancement (AIEE) Properties of Cyano-Stilbene Derivatives

한가람, 김영미

단국대 화학과

Most often the aggregation of π-conjugated organic chromophores with a planar and rigid structure induce a remarkable decrease of fluorescence efficiency in comparison with that of dilute solutions. This undesirable optical properties in the condensed state generally attributed to intramolecular and intermolecular interactions, which enhance the nonradiative deactivation process. Recently, however, several exceptional organic materials having enhanced emission rather than fluorescence quenching in aggregates or solid states have been reported. Such enhanced emission in solid state, which is called AIEE, has drawn considerable interests due to various potential applications including the fluorescent biological probes, optical sensors and light-emitting diodes (LEDs). We will present the synthesis of AIEE active materials and their detail photophysical properties in diluted solution and aggregate states and discuss the structural factors which induce AIEE characteristics.

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Synthesis and Photophysical Properties of a BODIPY-Based Environment-Sensitive Probe

곽민정, 김영미

단국대 화학과

Environment-sensitive fluorophores whose optical properties are dependent on surrounding environment have been widely used in a variety of biological applications such as protein-protein interactions, monitoring ions/H+ and polarity of microenvironment. We have synthesized BODIPY-based environment-sensitive fluorophore, which exhibits valuable optical properties as a biological probe. For example, the probe shows a blue shifted emission band in nonpolar environment with enhanced quantum yield in comparison with that in polar solvent. We will demonstrate the application of environment-sensitive probe for the detection of bovin serum albumin (BSA).

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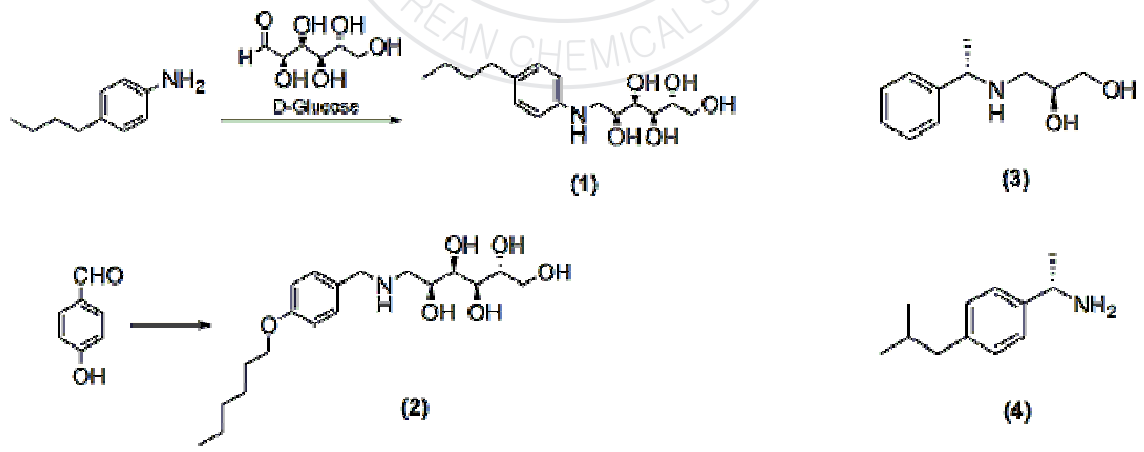
The synthesis of chiral amines for the resolution of (+),(-)-ibuprofen

이준엽, 이학준

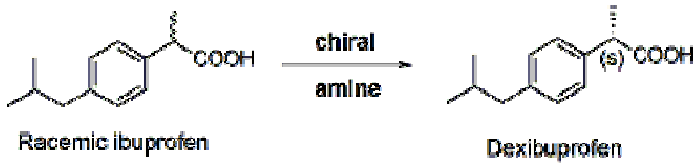
한양대 응용화학과

Ibuprofen, α-methyl-4-(2-methylpropyl)benzeneacetic acid, is well-known as antipyretic, and analgesic agent, non-steroidal anti-inflammatory drugs(NSAIDs). Dexibuprofen is (S)-enantiomer of Ibuprofen. It is known for its restrainable effect of in vitro synthesis of Prostaglandin which is a 160-fold more active than (R)- enantiomer's. In order to resolve (S)-ibuprofen we have synthesized three chiral amines. We will discuss the synthetic routes and the chiral resolution results in this presentation.

***Synthesis of Chiral amine**



***Resolution**



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Fluorescent chemosensors bearing pyrene derivative for the detection of DNA

정용숙

이화여대 바이오융합과

The synthesis of fluorescent chemosensors containing pyrene groups has recently emerged as a significant goal of research programs due to its distinctive monomer and excimer emissions. In addition, recognition and sensing of DNA using polyamine is of paramount significance because polyamines are positively charged and interact with negative charges like phosphate groups in DNA. We synthesize pyrene containing molecular systems bearing different length of poly amine linkers which show switching the monomer/excimer emissions that selectively respond to DNA in aqueous solution. Different fluorescent changes due to the bases were further confirmed and explained by UV absorption changes, CD experiments as well as intercalator displacement experiments. Few examples of pyrene derivatives and their fluorescence changes by external inputs will be proposed.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Colorimetric and Fluorometric Sensor for Lead Ion Based on Conjugated Polydiacetylenes

이경미, *윤주영

*이화여대 바이오.융합대학원 *이화여대 화학과*

University, Seoul 120-750, Korea.Pb2+ is considered as a toxic heavy metal ion because of the adverse health effects of lead exposure. It is reported that symptoms of lead exposure are memory lose, irritability, anemia, muscle paralysis mental retardation. Since sophisticated detecting methods for lead, there is a strong demand to develop a simple method for lead detection. Even though considerable efforts have been devoted to developing fluorescent chemosensors for various metal ions over the last few decades, there have been relatively less reports on Pb2+ selective fluorescent chemosensors. Compared to lead selective fluorescent sensors, there are only few examples of lead selective colorimetric sensors and even less examples of colorimetric sensors are available which work in aqueous solution. Certainly, naked-eye detection is the simplest way, which can find various applications for environmental purpose.Recently polymer based sensors have been intensively studied. Among them, polydiacetylenes (PDAs), a family of conjugated polymers, are very intriguing materials in several aspects. PDAs display an intense blue color and the blue PDAs can undergo a color shift to a red phase upon environmental stimulation. The stimulus-induced apparent blue-to-red transition of the PDAs has led to the development of a variety of PDA-based chemosensors. Herein, we report the first example of lead selective PDA-based chemosensor. In 100% aqueous solution, the presence of lead can be easily monitored via naked-eye detection. In addition, the fluorescence enhancement was observed upon the addition of lead ions.

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Napthoimidazolium-ammonium fluorescent receptors for ATP and GTP in aqueous solution of physiological pH

송나리, *윤주영

*이화여대 바이오융합과학대학원 *이화여대 화학과*

Recognition and sensing system based on anion-induced changes has recently been regarded as a key research field due to its significant roles in chemical and biological processes. In spite of considerable efforts for developing chemosensors for anions, there have been relatively few reports on various nucleoside triphosphate-selective receptors. Because it is still a challenging task to discriminate a certain nucleoside triphosphate among the others such as ATP, GTP, CTP, UTP, and TTP. Especially, ATP is a multifunctional nucleotide, known as the universal energy currency in all of the biological systems and a signaling molecule to coordinate responses to energy status. we have focused on synthesis of particular receptors bearing two or more napht hoimidazolium-ammonium groups for ATP and GTP by virtue of formation of strong $[C\text{-}H]^{+}\cdots X^{-}$ type ionic hydrogen bonding. This new water-soluble naphthoimidazolium derivative not only differentiates two structurally similar compounds GTP and ATP, but also acts as potential fluorescent chemosensors (as a quencher and an enhancer, respectively) for GTP and ATP in 100% aqueous solution (pH = 7.4, 20 mM HEPES). Their binding properties are presented herein using fluorescent study and NMR experiments.

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Two Novel Binaphthyl-Dimer Derivatives for Fluorescent Sensors

Wang Fang

이화여대 화학.나노과학부

Sensors based on the ion-induced changes in fluorescence have been actively investigated due to the simplicity and high detection limit of the fluorescence. Two novel binaphthyl-dimer-based fluorescent sensors, bearing pyrene groups via imine linkage, (PBD-1, PBD-2) were synthesized. PBD-1 exhibited a highly selective and significant fluorescence enhancement and colorimetric change towards Zn^{2+} among all the metal ions examined. The PBD-1-Zn^{2+} complex were successfully applied to detect Pi ($HPO4^{2-}$) in 100% acetonitrile. For further study, PBD-2, which is the reduced form of PBD-1, was investigated as a fluorescent chemosensor for the chiral anion recognition. These results showed that PBD-2 displayed an excellent chiral selectivity for D-alanine derivative.

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Conjugated Polydiacetylenes Bearing Imidazolium Groups

전혜령, *이경미, **윤주영

*이화여대 화학나노과학 *이화여대 바이오.융합대학원 **이화여대 화학과*

Polydiacetylene(PDA) is a colorimatric polymer that undergoes blue to red transformations in response to various biological analytes and processes. Due to its optical properties, PDA is an ideal choice for use as a chemosensor. PDA has been extensively investigated as a sensor matrix, due to a brilliant blue-to-red color transition that takes place in response to environmental perturbations, like temperature changes, pH, and surface pressure. It already has been known that “blue-phase” PDAs are nonfluorescent while their “red-phase” counterparts fluoresce. PDA is made by 1,4-addition between neighbored diacetylenic monomers, initiated by ultraviolet(UV) irradiation. The polymer which is formed by exposure to UV irradiation is intensely blue to the eye, because of electronic delocalization within the conjugated framework, generating absorption at around 650nm in the visible region to electromagnetic spectrum. In the current study, we prepared new PDAs bearing imidazolium groups and application of these polymers as chemosensors will be presented.

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Novel Binaphthyl-Containing Bi-Nuclear Complex with Low Concentration Quenching Effect for Efficiency Organic Light-Emitting Diodes

정지영, *Zhou Ying, **김장주, ***윤주영

*이화여대 바이오융합과학대학원 *이화여대 화학.나노과학부 **서울대 재료공학부 ***이화여대 화학과*

Significant progress has been made in organic light-emitting diodes (OLED) for display and solid-state lighting applications over the past few decades. Some organic fluorine-boron complexes, as the analogues of BODIPY (dipyrro-boradiazaindacenes), have been reported to achieve high solid state emission intensity or be promising electron transporting materials in OLED. Consequently, there has been increasing interest in the development of novel Boron complexes with a well-designed structure to overcome the weakness of BODIPY as well as control the optical properties, improve their electron-accepting capability and apply them successful with high-efficiency. In the design of the target molecule, bi-nuclear Boron complex centers were introduced to ensure strong fluorescence intensity and electron-transporting property. A highly efficient yellow emitting material (CMB1) based on a novel bi-nuclear Boron complex using the binaphthyl unit as the fluorophore. CMB1 showed low concentration quenching with a photoluminescence quantum yield of 10% in the solid state as well as good electron transporting ability. A combination of the electron transporting ability and low quenching concentration of the CMB1 provides OLEDs with unique opportunities due to the rarity of material systems that possess both properties simultaneously.

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Synthesis of Di-spirohydantoins and Benzyne Chemistry

장가영, 송주현, 이용균, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

A series of tropane and nortropane 3-spiro-5-hydantoins showed anticonvulsant activity against pentylenetetrazol-induced convulsions in mice and antiarrhythmic activity in rabbit previously treated with ouabain. We already reported the synthesis of N-substituted 8-azabicyclo[3.2.1]octan-3-ones dervatives and novel spirohydantoin derivatives by using N-substituted 8-azabicyclo[3.2.1]octan-3-ones. As a part of a research program related to the synthetic study of pharmacologically interesting tropane compounds, we now report the synthesis of corrsponding novel dispirohydantoin derivatives by using di-(8-azabicyclo[3.2.1]octan-3-only)alkanes with potassium cyanide and ammonium carbonate. We will try reaction of amines and 2.5-dimethoxytetra hydrofuran with 2-(trimethylsilyl)phenyltrifluoromethansulfonate.

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Synthesis of 1,5,3,7-Diazadiphosphocine and metal complex

이은수, 이도훈, 최순규, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

Great efforts have been devoted to the development of efficient ligands for transition metal, in order to obtain complexes whose stability, physical properties, and biodistribution could make them suitable for application as contrast agents for magnetic resonance imaging (MRI), diagnostic-therapeutic radiopharmaceuticals, or fluorescent bioassays. We now report reaction of the amino acids (or amines) with hypophosphorous acid and form-aldehyde. And we executed reaction of 1,5-diphenyl-3,7-dihydroxy-3,7-dioxoperhydro-1,5,3,7-diazadiphosphocine by using metal film.

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Diketone Synthesis from 4,4'-Diiodobiphenyl and Arylboronic Acid with Carbon monoxide (or Metal carbonyl)

신은혜, 송주현, 김윤영, 최순규, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

Terphenyl derivatives have been known to exhibit a variety of optical and electrical properties. Naturally isolated *p*-terphenyl metabolites are known to possess the potent biological activities. In our ongoing studies endeavored toward wittig reaction of diketone formed by Suzuki carbonylative reaction with aryl ylide to afford stilbene derivative. We exected 4,4'-diiodobiphenyl and arylboronic acid with carbon monoxide (or metal carbonyl) via Pd(NHC) complex. Synthesyed diketone products are biphenyl-4,4'-diylbis(phenyl-methanone) and biphenyl-4,4'-diylbis(naphthalen-1-ylmethanone).

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장소: 대구엑스코
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

An efficient One-pot Reaction of amines with 2,5-dimethoxytetrahydrofuran in acid solution and Benzyne chemistry

정수경, 이언진, 이용균, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

Nitrogen containing heterocycles, such as pyrroles, indoles and carbazoles have attracted considerable attention due to their numerous applications in pharmaceutical and synthetic chemistry. Especially, a series of tropanes showed anticonvulsant activity against pentylene-tetrazol-induced convulsions in mice and antiarrhythmic activity in rabbit previously treated with ouabain. As a part of a research program related to the synthetic study of pharmacologically interesting tropane compounds and nitrogen containing heterocycles, we now report a convenient one-pot sythesis of tropane compounds and nitrogen containing heterocycles in the reaction of amines(or phosphoramidates) with 2,5-dimethoxytetrahydrofuran, and actonedicarboxylic acid at 0℃ (on reflux). And we tried reaction of amine, 2,5-dimethoxytetrahyrofuran, and 2-(trimethylsilyl)phenyl trifluoromethanesulfonate in acid solution.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Turn-On Fluorescent Chemosensor for F^- Based on Pyreneamide Derivative

전남중, 홍성원, 홍주현, 남계춘

전남대 화학과

Fluorescent chemosensors can be effectively used as a tool to analyze and clarify such roles of charged chemical species in living system as well as to measure the amount of ions from the sources contaminated with them. Among fluorophores, pyrenes are known as one of the most useful fluorogenic units because they display not only a well-defined monomer emission at 375 nm. The pyreneamide derivative was obtained successfully by the reaction of bipyridine with 1-pyrenemethylamide. Pyreneamide derivative has nearly no fluorescence in acetonitrile solution. However, in the presence of fluoride ion, a turn-on fluorescence was observed. Other ions in solution show very little emission.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Metal ion Templated rotaxane Formation with RCM

홍성원, 전남중, 정주미, 남계춘

전남대 화학과

Rotaxanes attract a great deal of attention because of their potential for applications in mesoscale devices and molecular machinery on the nanoscale. The synthesis of these interlocked systems usually requires the recognition of a macrocyclic unit by a recognition. The rotaxane is particularly notable examples that have been used to construct several molecular switches because they can recognize several guests. Our approach has been to bring together neutral marcrocyclic component and containing pyridinium axles to creat rotaxane. The rotaxane binding properties investigated with ,^{1}H-NMR titration methods with various metals.

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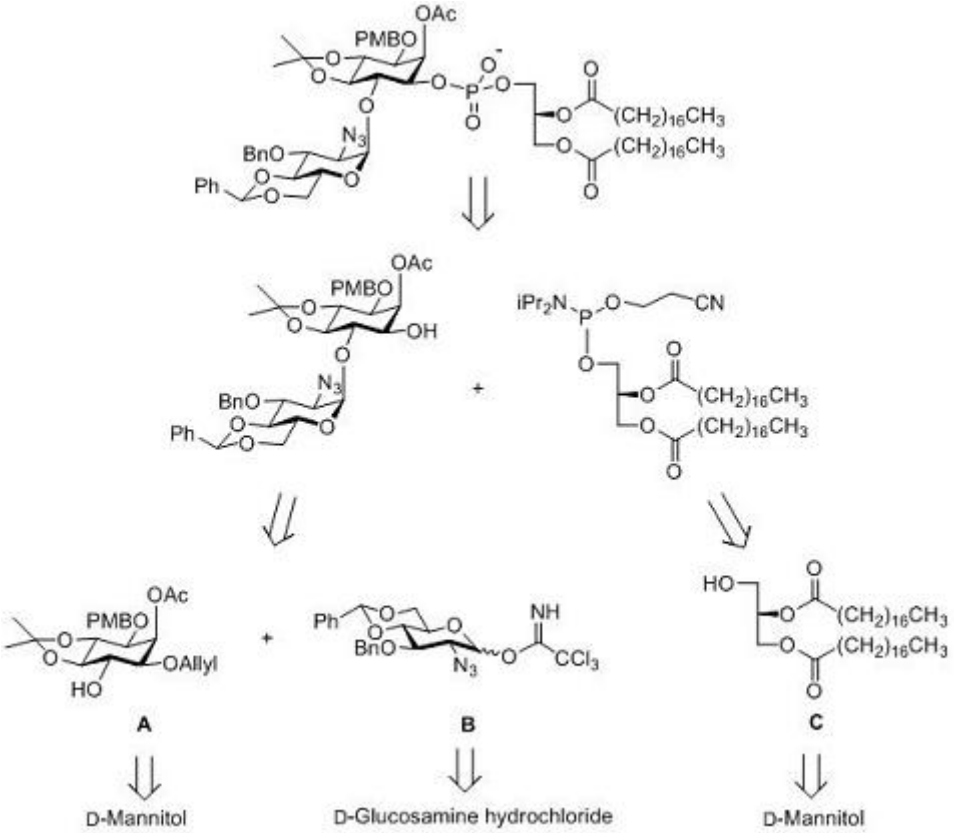
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Stereoselective Synthesis of the $GlcNH_2$-Inositol-Lipid Part in the Glycosyl Phosphatidyl Inositol Anchor of *Scrapie* Prion Protein

강현구, *김관수

*연세대 화학 *연세대 화학과*

The mad cow disease (MCD) is a fatal, neurodegenerative disease in cattle, which generates spongy in the brain and spinal cord. A lot of scientists guess the disease as transmittable to human being by taking the brain and spinal cord of infected cattle. In an effort to study significant biological functions of the MCD and to develop the chemotherapy agents, it is vital to synthesize the glycosyl phosphatidyl inositol (GPI) anchor, which connects *scrapie* prion protein via their C-terminus to eukaryotic cell membranes. In the present work, the synthesis of a properly protected form of the $GlcNH_2$-Inositol-Lipid part in the GPI anchor of *scrapie* prion protein was achieved. A pseudodisacchride, $GlcNH_2$-Inositol, was synthesized by the α-selective glycosylation of a suitably protected *myo*-inositol A with 2-azidoglycosyl trichloroacetimidate donor B. The protected *myo*-Inositol A was prepared from D-mannitol employing the ring closing metathesis. Then, the lipid part, which was obtained from D-mannitol, was connected to the pseudodisaccharide through *O*-1 of the *myo*-inositol.



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장소: 대구엑스코
발표코드: **ORGN.P-294**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

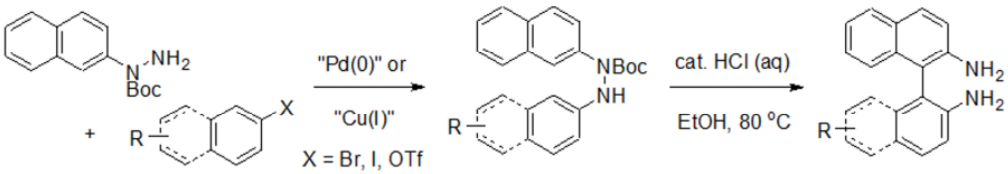
Acid-catalyzed [3,3]-sigmatropic rearrangement of *N*-Cbz-diaryl hydrazide for the synthesis of *N*-Cbz-1,1'-biaryl-2,2'-diamines

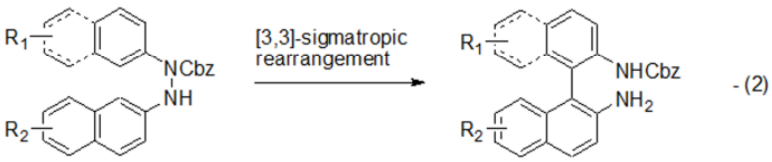
임병윤, 서성은, 박인걸, 조천규

한양대 화학과

Axially chiral biaryls are important structural motifs as versatile auxiliaries for various asymmetric synthetic transformations.

We have previously reported that diaryl hydrazides are effective surrogates of diaryl hydrazines, proceeding the acid-catalyzed [3,3]-sigmatropic rearrangement reaction to afford 2,2'-diamino-1,1'-biaryls (eq. 1, Scheme 1). Unlike diaryl hydrazines, the starting diaryl hydrazides are readily accessed from aryl hydrazide via the Pd(0) or Cu(I)-catalyzed coupling reactions with aryl halide. Prompted by our recent discovery that the Fischer indolization of *N*-Cbz-aryl hydrazide can proceed without the removal of *N*-protecting group, we set out to convert diaryl hydrazide into mono-*N*-Cbz-1,1'-biaryl-2,2'-diamines (eq. 2). As the free –NH2 group can be readily converted into other functionalities, mono-*N*-protected diamine would enable the generation of structurally and functionally diverse 1,1'-biaryls bearing either C2- or C1-symmetric biaryl backbone.





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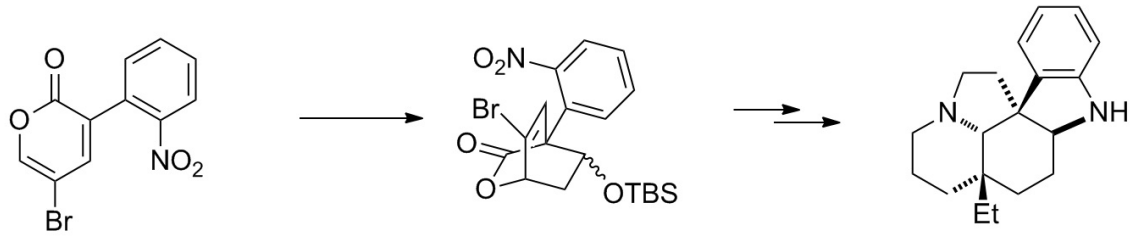
발표종류: 포스터, 발표일시: 금 15:00~17:00

Studies toward the total synthesis of (±)-aspidospermidine

조현규, 조천규

한양대 화학과

Aspidosperma alkaloid family comprises one of the largest groups of indole alkaloids with more than 250 members. Structurally, aspidosperma alkaloids share a common characteristic pentacyclic ABCDE framework where the central C-ring possesses all stereocenters and significant functional groups. Because of a wide range of intriguing biological activities portrayed by many of the members, a considerable research interest has been devoted in their synthesis, leading to the development of many efficient and elegant synthetic methods and routes. In order to explore the potential applicability of 2-pyrone Diels-Alder strategy to the target-oriented synthesis, we have investigated the total synthesis of aspidospermidine with the maximum use of the resultant densely functionalized cycloadduct. More importantly, our study would establish a platform for the synthesis of various other structurally related aspidosperma alkaloids including tabersonine, catharanthine, vindoline as well as aspidophytine. Herein, we report the preliminary account of our 2-pyrone strategy to the synthesis of the key framework of aspidosperma alkaloids.



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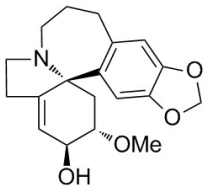
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Studies toward the total syntheses of (±)-homoerythratine and (±)-3-epi-schelhammericine

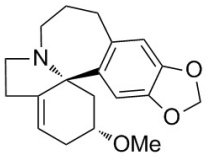
송지영, 조천규

한양대 화학과

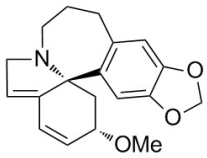
Widely distributed in the plant kingdom, the homoerythrina alkaloids are comprised of more than 70 natural products. Possessing an intriguing azatetracyclic framework in common, they are categorized into aromatic or nonaromatic D-ring subtypes. The former category is predominant and includes homoerythratine (1), 3-epi-schelhammericine (2), and 3-epi-schelhammeridine (3). The homoerythrina alkaloids are structurally similar and biosynthetically related to the Erythrina alkaloids (azacyclohexene C-ring vs azacycloheptene C-ring of homoerythrina alkaloids (5)). While many of the Erythrina alkaloids (4) exhibit various biological activities including curare and hypnotic effects, there are no reports on pharmacological effects of either homoerythratine or 3-epi-schelhammeridine, although the alkaloids extracted from leaves of the genus Dysoxylum lenticellare, assumed to contain 3-epi-schelhammericine was reported to have both cardiac effects in rats and molluscicidal activity. As a part of ongoing study exploring the potential of 2-pyrone Diels-Alder strategy to the target-oriented synthesis, we have envisaged both homoerythratine (1) and 3-epi-schelhammericine (2) could be readily forged from the cycloadducts of 3,5-dibromo-2-pyrone with the properly functionalized dienophiles. Herein, we report the preliminary account of the strategic use of our 2-pyrone Diels-Alder chemistry toward the total syntheses of the title alkaloids.



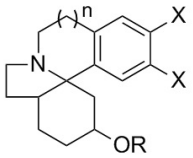
homoerythratine (**1**)



3-epi-schelhammericine (**2**)



3-epi-schelhammeridine (**3**)



4: n=1 *Erythrina* alkaloids
5: n=2 homoerythrina alkaloids

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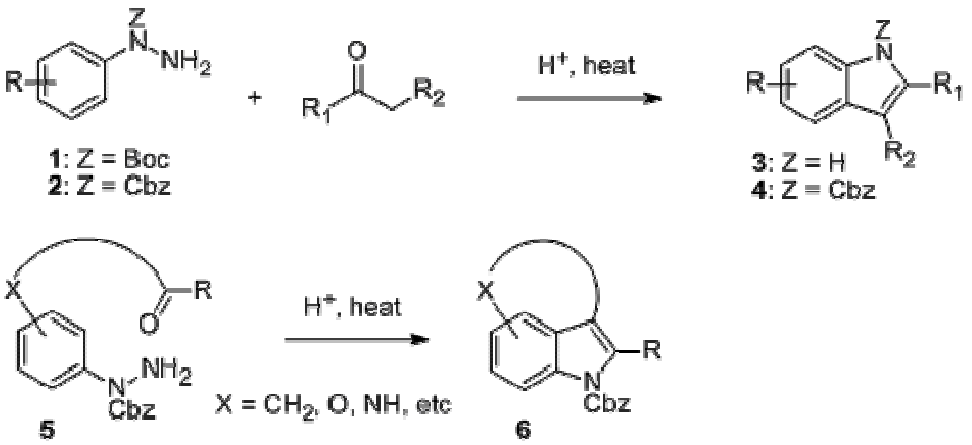
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Intramolecular Fischer indolization for the construction of tricyclic indole core of ergot alkaloids

박인걸, 조천규

한양대 화학과

We have previously demonstrated that aryl hydrazides 1 are effective surrogates of aryl hydrazines, undergoing the Fischer indolization reaction to afford the corresponding indoles, when treated with enolizable aldehydes and ketones in the presence of an acid (1 → 3). Unlike aryl hydrazines, the aryl hydrazides are readily accessed from aryl halides via the Pd(0) or Cu(I)-catalyzed coupling reaction with *N*-Boc hydrazine. We have also reported that *N*-Cbz-aryl hydrazide 2 can proceed in a Fischer indolization reaction to give *N*-Cbz-indole 4 without the elimination of *N*-Cbz group. Prompted by our recent interest on the synthesis of ergot alkaloids, we set out to study the intramolecular Fischer indolization reaction of the aryl hydrazide that are linked to carbonyl functions by various tether groups as a new synthetic means to the construction of tricyclic indole system (5 → 6).



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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Oxidation of benzoins to benzils by sodium hydride as oxidative agent

강선혜, 주천익, *김선민, 한호규, *양정운

*고려대 화학과 *성균관대 에너지과학과*

we have focused our attention towards the development of green reagent. Herein, we report that sodium hydride can be used effectively for the direct conversion of benzoins to benzyls under mild condition, which is of great value with respect to environmental and practical concerns. Sodium hydride is ordinarily employed as a strong base for deprotonation of amide, esters, stannanes and alcohols or as a reducing reagent for disulfides, disilanes, azides and isoquinoines.To develop a useful protocol, we first studied the reaction of benzoin with 2 equivalents of sodium hydride under a variety of conditions. The best chemical yield (>95%) was obtained when the reaction of benzoin is carried out in the presence of 2.0 equivalents of sodium hydride in THF at room temperature.we have demonstrated for the first time a facile and simple method for the oxidation of benzoins into benzils with sodium hydride as an oxidative agent, providing the corresponding products in good to excellent yields. Further studies of other related applications of this protocol are currently ongoing in our laboratories.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Combinatorial approach to the developement of Fluorescent Chemoensors for Metal Cations

이상욱

서울대 화학부

1. We developed first DOS fluorescent sensor library for metal cation detection, using metal chelators as combinatorial building blocks of styryl library. 2. The majority of library compounds showed fluorescent response to 5 transition metal cations (Zn2+, Cd2+, Hg2+, Pb2+ and Ag+). 3. Ultraselective sensors especially for Hg2+, Ag+ or Zn2+. These sensors could be applicable in selective cellular imaging of Hg2+. 4. The sensor's selectivity for metal cation was determined not by only receptors but also by fluorophore structure.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Organic thin film transistor using photo-curable organic/inorganic hybrid materials as a gate dielectric

김윤태, 황도훈

부산대 화학과

For the past ten years, organic materials have been extensively investigated as an electronic material for thin film transistor (TFT) devices. Organic materials offer strong promise in terms of properties, processing and cost effectiveness and they can be used in flat panel displays, smart cards and large area electronic applications. The present, organic semiconductors and metals required for OFETs were improved considerably. However, in the case of dielectric, not many researchers have been done. Here we synthesized polyhedral oligomeric silsesquioxane (POSS)-based insulating materials with acryl functional groups. The insulators were curable by UV irradiation in presence of selected photo radical initiators. We fabricated MIM device of ITO/insulator/Au to measure electrical properties such as current density, capacitance. We fabricated an organic thin film transistor with pentacene as the p-type material and the photo-curable POSS derivatives as an insulator. The pentacene transistor with the insulator layer shows comparable transistor characteristics as that with the prototypical polymeric gate insulator of poly (vinyl phenol) (PVP).

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Organic Dyes Containing Phenothiazine Derivertives

곽영우

경북대 화학과

The interest in metal- free organic dyes with high extinction coefficients has grown in recent years. In this presentation, we report synthesis and application of new organic dyes. The organic dyes contain multiple electron donor chromophore groups (phenothiazine,carbazole, triphenylamine, dimethylaniline) and acceptor groups (cyanoacetic acids, rhodanine-3-acetic acid). The performances (Isc, Vsc, ff, IPCE, PCE) of the DSSCs using the dyes are evaluated. Results show that the distributions of HOMO and LUMO orbitals of dyes are completely separated, indicating that photo excitation may lead to an efficient intramolecular charge separation with an effective photocurrent generation and the solar energy-to-elecricity conversion efficiency(η) of dyes containing a N-hexylphenothiazine as an electron donor chromophore which is connected to an electron acceptor such as cyanoacetic acid are better than that of a N-hexylcarbazole as an electron donor chromophore.

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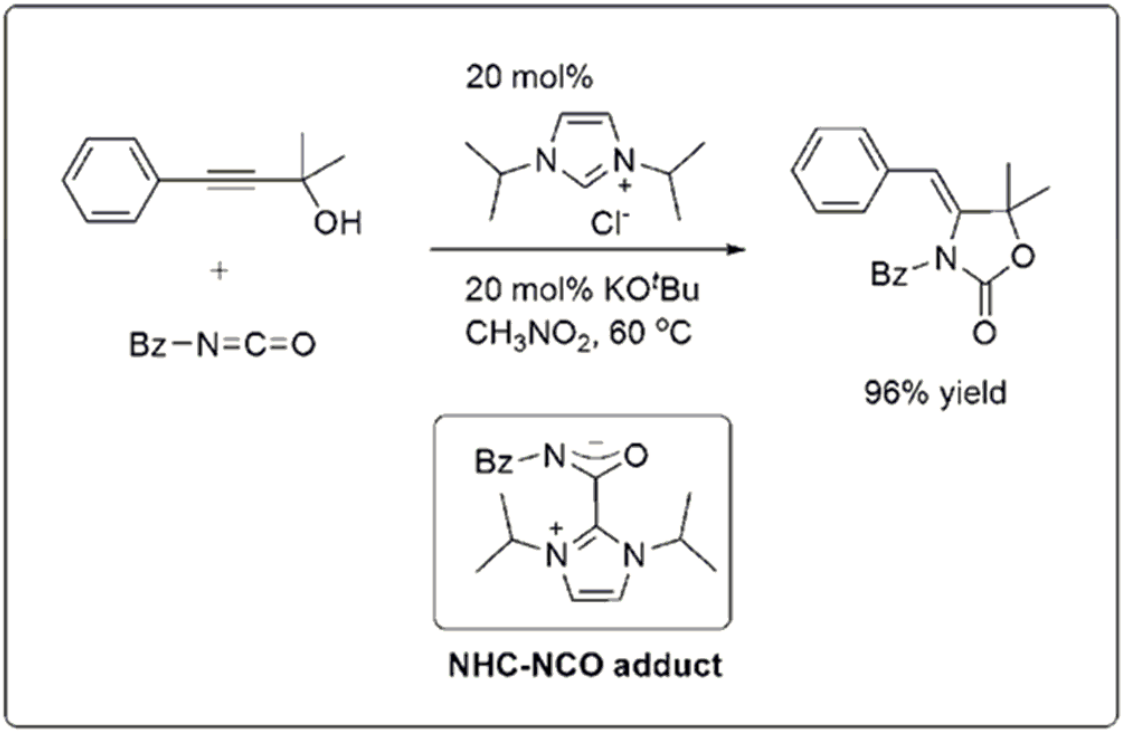
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

N-Heterocyclic carbenes as efficient organocatalysts for the synthesis of 4-methyleneoxazolidin-2-one

조경아, *강은주

*경희대 화학과 *경희대 응용화학과*

The catalytic activity of NHC is probed in the coupling reaction of isocyanates and propargylic alcohols to afford heterocyclic organic compound. Most NHC-mediated organocatalysis includes the formation of covalent, active intermediates by their addition to C=O bonds as the key step. Such an apparent donor character of NHCs has also been applied to isocyanate, and the resulting intermediates are identified as the zwitterionic NHC-NCO adducts. The oxazolidinone formations from propargylic alcohols using the NHC-NCO adduct can be explained by a mechanism involving the nucleophilic addition of the imidazolium-isocyanate adduct to the alkyne and subsequent intramolecular cyclization of alkoxide intermediates. The positive effect of the electron-donating alkyl substituents on the NHC nitrogen atoms implies that the nucleophilic attack of the NCO moiety, bound to the NHC, onto the substrates is a possible rate-determining step in the catalytic cycle. We have demonstrated that NHCs and NHC-NCO adducts serve as potent organocatalysts providing straightforward methods for 4-methyleneoxazolidin-2-one synthesis.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Pd-CNT nanocomposites and its application for the Mizoroki Heck reaction and Sonogashira reaction

박아별, Thiruvengadam Palani, 이선우

전남대 화학과

Recently, carbon nanotubes (CNTs) have received 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 CNT-supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibiting good catalytic behaviors under various chemical reaction conditions, involving methanol electro-oxidation, selective hydrogenation, Suzuki coupling, CO oxidation, and Fischer-Tropsch synthesis. However, few studies have centered upon CNTs as catalyst supports for hydrodehalogenation reactions, a key approach in preventing environmental pollution. A catalytic system based on Pd-CNT nanocomposites for the Mizoroki Heck reaction and Sonogashira reaction of aryl halides is developed. Thiol groups were utilized as linkers to secure the Pd nanoparticles without agglomeration. The Pd-CNT nanocomposites effectively promoted the Mizoroki Heck reaction and Sonogashira reaction of aryl halides at a low Pd content (~ 2.3%) 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 Mizoroki Heck reaction and Sonogashira reaction.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of Diaryl alkynes from propiolic acid by using palladium catalyst

박경호, 이선우, 박남진, manian rajesh kumar

전남대 화학과

In order to synthesize unsymmetrically substituted diaryl alkynes using the Sonogashira Decarboxylative coupling of sp-sp2 carbon is possible by palladium-catalyst. Employing propiolic acid as a difunctional alkyne, and using consecutive reactions of the Sonogashira reaction and the decarboxylative coupling, unsymmetrically substituted diaryl alkynes were obtained in moderate to good yield. 2-Octynoic acid and phenylpropiolic acid were employed for the palladium-catalyzed decarboylative coupling reaction and with a variety of aryl halides. The former needed dppb as a ligand, the latter tri-t-butylphosphine. These reactions showed high reactivities and tolerance of functional groups such as vinyl, ester, ether, ketone, and amine. Symmetric diarylalkyenes were obtained from the decarboxylative coupling reaction of propiolic acid (or 2-butynedioic acid) and aryl halides in good yields. In addition, unsymmetric diarylalkynes were synthesized from the reaction with propiolic acid, phenyl iodide and aryl bromides. They showed tolerance toward functional groups such as ester, ketone and aldehyde, and exhibited chemoselectivity. This work illustrates two conceptual advances. First, as this eco-friedly method does not require organometallic reagents such as silyl or tin-protected alkynes, it does not produce toxic organometal waste. In addition, it does not need copper as a cocatalyst, and produces CO2 as a byproduct. Second, this method is economical and has easy handling. It does not need an excess of base with only 2 equivalents of 1,8-diazabicyclo[5.4.0]udec-7-ene (DBU), which is cheaper and more stable than the previously used TBAF, being needed. 1,4-(Bisdiphenylphosphino)butane, which could be handled in air and is more stable than PtBu3, was employed as a ligand and showed good activity. Therefore, the proposed, eco-friendly, economical and simple handling system makes this process superior to existing processes. Moreover, 2-butynedioic acid also showed good reactivity as an alkyne source. In addition,

this catalytic system afforded the desired coupled product under water condition, exhibited very good reactivity in the microwave system.

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Palladium-Catalyzed Mizoroki-Heck Coupling Reactions Using Sterically Bulky Phosphite Ligand

정은혜, 김용, 이선우

전남대 화학과

Palladium-catalyzed carbon-carbon bond forming reactions have received much attention in research into organic synthesis for decades. Like other type of palladium-catalyst coupling reactions, Mizoroki-Heck reaction's activity is also highly dependent on the nature of the ligand, for example, its electronic and steric effect. Recently, sterically bulky monodentate phosphine and N-heterocycle carbene have been developed and afforded high activity. However, alkyl phosphine ligands are not stable toward oxygen and moisture, and most of the N-heterocylce carbene ligands required a cumbersome synthetic step. To overcome these problems, we have examined sterically bulky phosphite ligands. A new catalytic system based on palladium-phosphite for Mizoroki-Heck coupling reactions of aryl iodide and bromide is described. An air-stable phosphite ligand afforded the desired products with high yields in the palladium-catalyzed Mizoroki-Heck reactions. The coupling of aryl iodides was optimized with 0.5 mol% Pd(OAc)2, 1 mol% phosphite, and K2CO3 in DMF solvent. For the coupling of aryl bromides, 1 mol% Pd(OAc)2 and 5 mol% phosphite were required with Na2CO3 as base. As a coupling partner alkene, n-butyl acrylate, t-butyl acrylate, styrene and N-t-butyl acrylamide all showed good yields.

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Novel (*R*)-Lipoic acid-dopamin hybrid molecules for cholinesterase inhibitor

우연지, *연고흠, 김현주, **고장면, **이봉호, **박정호

*한밭대 응용화학 생명공학과 *한밭대 응용화학과 **한밭대 응용화학생명공학부*

(*R*)-Lipoic acid(LA) is a natural antioxidant and cofactor of several enzymes. Our group has been interested in molecular hybridization between bioactive natural compounds. A series of lipoic acid-dopamin derivatives using dopamin, 5-methoxytryptamine, and tryptamine were synthesized as potential cholinesterase inhibitor. *In vitro* cholinesterase inhibition activities [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] of the hybrid compounds were checked. Some hybrid molecules had lower IC_{50} value than the single parent compound as a cholinesterase inhibitor. Specifically, LA-5-methoxytryptamine and LA-tryptamine were shown as an effective inhibitors of BuChE and also had a great selectivity for BuChE over AChE.

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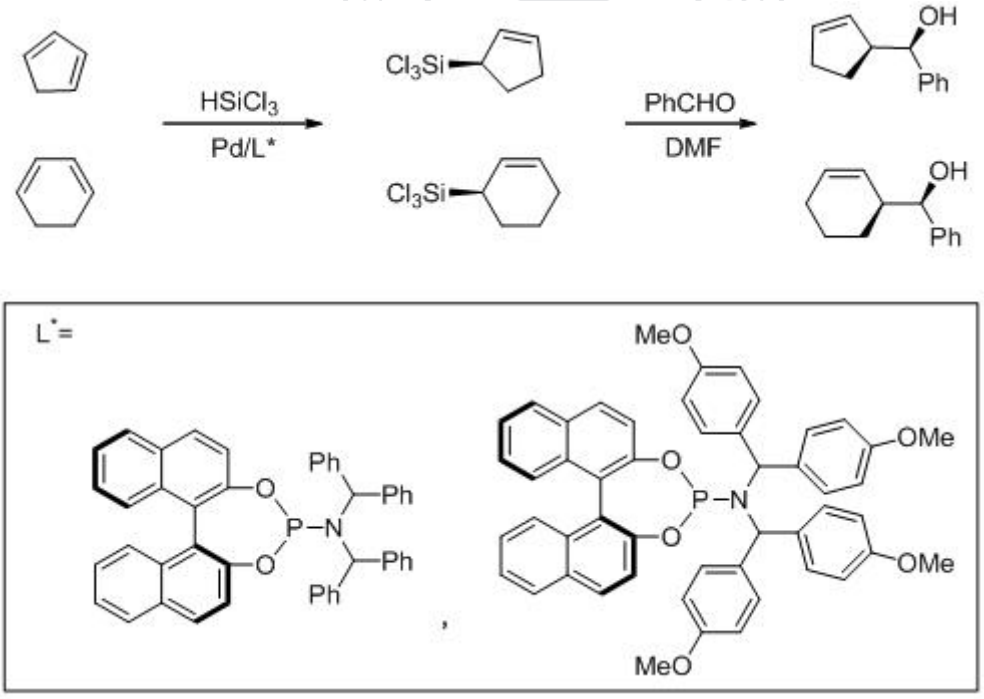
Palladium-Catalyzed Asymmetric Hydrosilylationof Cyclic 1,3-dienes with Chiral Phosphoramidite Ligands

유호정, *박훈서, *한진욱

*한양대 화학 *한양대 화학과*

Palladium-catalyzed asymmetric hydrosilylation of olefins provides one of the most efficient routes to optically active allylsilanes, which are able to be further derivatized to useful synthetic intermediates such as allyl alcohols and homoallyl alcohols. Chiral phosphoramidite ligands, containing an axially chiral BINOL and a bulky amine, were applied to palladium-catalyzed asymmetric hydrosilylation of cyclic 1,3-dienes in this study. Enantioselectivities were varied dramatically according to the chiral ligands used.



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Isolation and Synthesis of Bacterial Culture Broth Metabolite N-(4-Oxopentyl)Acetamide

Md.Maniruzzaman Manir, V.S.Jamal Ahamed, 이민경, 문석식, *박경석

*공주대 화학과 *농촌진흥청 국립농업과학원 농업미생물과*

Bacillus vallismortis strain EXTN1 was originally isolated from red pepper and has been worked as an efficient plant growth promoting and diseases controlling agent. A chemical investigation of the methanolic extract of EXTN1 led to the isolation of N-(4-oxopentyl)acetamide through a series of silica gel column chromatography and preparative C-18 HPLC. Its structure was determined by spectroscopic methods including IR, UV, HRTOFMS, and 1D & 2D NMR and conformed by synthesis from 5-Chloropentanone. Isolation and the reaction will be presented.

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Synthesis and Characterization of New Anthracene-Based Blue Light Emitting materials

이민정, 강문성, 배만훈, 김철영, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

OLEDs have attracted a great deal of attention because of their promising applications in full-color flat-panel displays, In OLED, there basic colors, red, green, and blue, are needed for a full-color display. Among three colors, it is much difficult to produce a blue emission, Anthracene has aromaticity which makes thermal, electrochemical properties stable. In the present work, we report on the design, synthesis, and characterization of blue light emitting material containing anthracene which is highly fluorescent and efficient chromophore.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Synthesis and characterization of a novel oligomer based on anthracene moiety for organic light-emitting diode

김철영, 이민정, 배만훈, 강문성, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Organic light-emitting devices (OLEDs) have received a great deal of attention recently, due to their promising applications in emissive displays. Anthracene has a rigid ring structure which minimizes vibronic energy levels to give high color purity and efficiency. And various groups can be substituted to many positions. In this presentation, we report on the design, synthesis, and characterization of new anthracene-based blue-light-emitting material with asymmetric structure.

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Electrogenerated Chemiluminescent "Turn-On" Sensor for Homocystein and Cystein Based on a Cyclometalated Ir(III) Complex in Aqueous Solution

이경식, 홍종인

서울대 화학부

Cys and Hcy are essential biological molecules required for the growth of cells and tissues in living systems. The deficiency of Cys is associated with retarded growth, hair depigmentation, edema, lethargy, liver damage, muscle and fat loss, skin lesions, and weakness. An elevated level of Hcy in human plasma is a risk factor for Alzheimer's, cardiovascular diseases, neural tube defect, inflammatory bowel disease, and osteoporosis. Therefore, the selective detection of Hcy and Cys in human blood plasma is very important and can be useful as a various disease-associated biomarker. Herein, we report a sensing strategy where an organometallic probe undergoes selective chemical reaction with homocystein (Hcy) and cystein (Cys), and then it subsequently produces efficient emission by electrochemical triggering. This approach which exploits the electrogenerated chemiluminescence (ECL) upon the selectively chemical reaction between a synthesized Ir(III)complex. This sensor shows selective response to Homocysteine(Cysteine) and Cysteine(Cys) over other various amino acids and thiol biomacromolecules in acqueous solution(CH3CN/H2O).

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Total Synthesis and Stereochemistry of Mycolactone F

김한제, *Yoshito Kishi

*공주교육대 과학교육과 *Department of Chemistry and Chemical Biology, Harvard University, U.S.A.*

Buruli ulcer is a severe necrotizing skin disease caused by Mycobacterium ulcerans. In 1999, Small and coworkers isolated the toxic metabolites, named mycolactones A and B, from M. ulcerans. Evidence from animal studies suggested that mycolactones A and B are directly responsible for the observed pathology. Recently, a mycolactone congener, called mycolactone F, was isolated from the fish pathogen M. marinum, and its gross structure was proposed. Intriguingly, mycolactone F was reported to exhibit a significantly lower toxicity. The mycolactones have attracted considerable attention from the synthetic community not only for their highly potent biological activity but also for being the first examples of polyketide macrolides to be isolated from a human pathogen. In this poster, we describe the total synthesis and the stereochemistry assignment of mycolactone F.

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Discrimination of regioisomers by charge transfer complexation in cucurbit[8]uril

조승원, 강민수, 정원석, 강민경, *오진호, **김민경, **이미희, **김희준

*한국과학영재학교 *KAIST 과학영재교육연구원 **금오공과대 응용화학과*

The charge-transfer (CT) interactions or donor–acceptor interactions between π-systems are an important class of non-covalent interactions and have been greatly exploited in the design and synthesis of self-organizing systems. Since the first example of selective inclusion of an electron-donor and -acceptor pair in cucurbit[8]uril, driven by the strong CT interaction between the guests was reported, the host-stabilized CT complex formation has been offered new opportunities to construct supramolecular assemblies. We here present that the formation of supramolecular CT complexes in CB[8] can be utilized to discriminate regio isomers of electron donor guest molecules.

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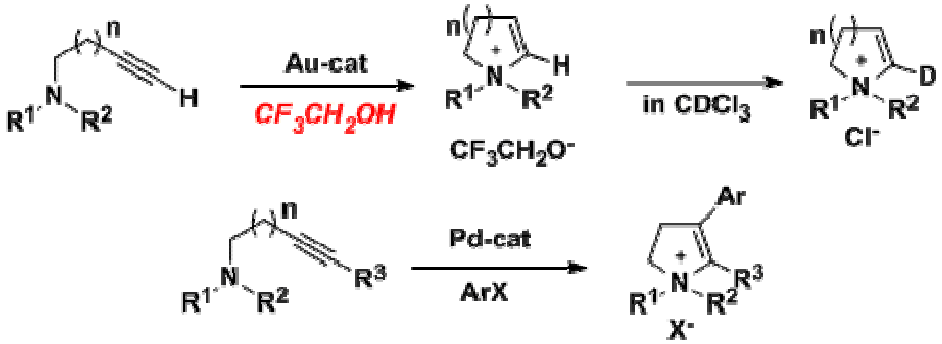
Synthesis of N-Quaternary Ammonium Salts Catalyzed by Gold-and Palladium Complexes

이연건, 박현섭, 신승훈

한양대 화학과

Hydroamination has attracted considerable attention as a direct, atom-economical means of C-N bond construction. Although catalytic addition of N-H bond onto alkene or alkyne has been well investigated, the addition of tertiary amines onto unpolarized unsaturated bonds to form ammonium salt has not been investigated well. In view of recent surge of phase transfer catalysis mediated by chiral N-quat salts, it is highly desirable to have a concise access to structurally diverse ammonium salts. However, a catalytic process of non-substitution type has not been possible in the realm of cross-coupling reaction, presumably due to the enthalpic penalty. We report herein two catalytic protocols for the formation of N-quaternary ammonium salts via intramolecular addition of tertiary amines onto alkynes. We found that the gold catalyzed addition of tertiary amines onto alkynes is highly dependent on the pKa of the solvent and appropriate balancing the acid-base property of the substrate-solvent led to a concise access to ammonium salts of various types proceeding at rt. Some of the preliminary studies on the derivatization at the alpha-position (to N-atom) will also be discussed. Alternatively, palladium catalyzed oxidative addition, aminopalladation, reductive elimination sequence provides N-quaternary ammonium salts having substituents at the beta-position.



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Coordination of pyridine-cored dendron on zinc porphyrin-cored dendrimers

신은주, 최고은

순천대 화학과

Dendrimers with zinc porphyrin core could form the coordination complexes with pyridine via axial ligation. On complexing zinc porphyrin with an axial ligand, two effects are often seen in the UV-vis spectrum: a red shift of the entire spectrum relative to that of zinc porphyrin and an increase in the εα/εβ ratio of the two visible bands. Thus, one could use the wavelength shift and intensity ratio of the visible bands as a measure of the degree of complexation. Construction of higher-dimensional dendrimer may be possible by the formation of coordination complex between dendrimers of different type, such as coordination of pyridine-cored dendron on zinc porphyrin-cored dendrimers. In the presence of pyridine-cored dendron, the complexation of zinc porphyrin-cored dendrimer results in the red shift of Soret band and Q band maxima, and the increase of the intensity ratio εα/εβ with red-shift of fluorescence maxima. This study deals with the preparation of various zinc porphyrin-cored dendrimers and how the dendritic environments of zinc porphyrin-cored dendrimers affect the axial coordination of pyridine as a model of high dimensional porphyrin dendrimer.

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Preparation, Characterization, and Photochromic Properties of Zinc Porphyrin- Spiropyran Dyad

신은주

순천대 화학과

Zinc porphyrin is one of most frequently employed photoactive molecules due to its spectral and redox properties. Numerous research groups have designed and prepared the molecular energy storage devices containing porphyrin moiety. Spiropyran is well-known photochromic compound accomplishing molecular structural change to merocyanine form by ring opening on UV irradiation. In turn, merocyanine is transformed to spiropyran by ring closure on irradiation of visible light Reversible photochromic spiropyran-merocyanine transformation is one of the subject of active research on optical memory and switch. Incorporating photochromic molecules into organic materials leads to photoresponsive systems, the properties of which can be manipulated by light. Because absorption spectra of two isomeric molecules are significantly different, the color change is the most spectacular evidence of photochromism. Besides this color change, many molecular and bulk properties also change in the case of incorporating photochromic molecules into organic materials. In this study, Zinc porphyrin-spiropyran dyad was prepared and the photochromic behavior was investigated.

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Aluminum amide mediated synthesis of oxalyl bis-amide

이영석

대구가톨릭대 화학과

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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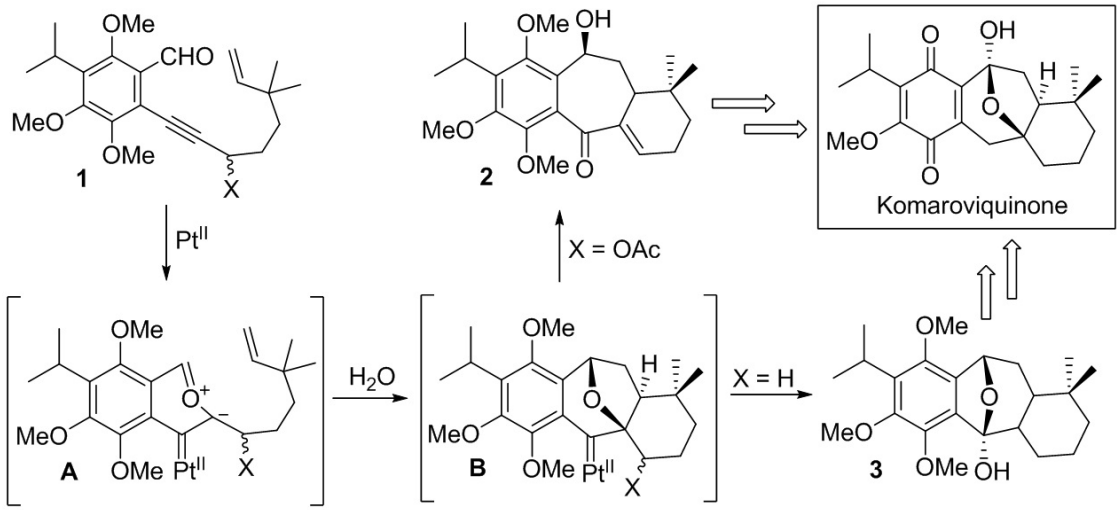
Pt-catalyzed Hydrative Cyclization of 2-(7-En-1-ynyl)benzaldehydes and its Application to Komaroviquinone Synthesis

이지호, **PIAOLANHUA**, 오창호

한양대 화학과

Discovery of new and efficient synthetic routes towards polycycles containing a central 7-membered carbocycle is still a challenging task to organic and medicinal chemists because many 7-membered ring containing polycycles have been isolated in recent years and some of them turned out to be biologically active natural products. During the course of our scientific endeavors leading to a general and modular entry to seven-membered ring-containing natural products, we observed a highly unique behavior of Pt-carbene complexes (B), which would subsequently undergo hydration to afford the tricyclic products in good yields with excellent stereoselectivities. This hydrative cyclization can be applied to the Komaroviquinone synthesis (Scheme 1).



Scheme 1. Pt-Catalyzed Cyclization of 1 via Pt-carbene complex ***A*** and **B**.

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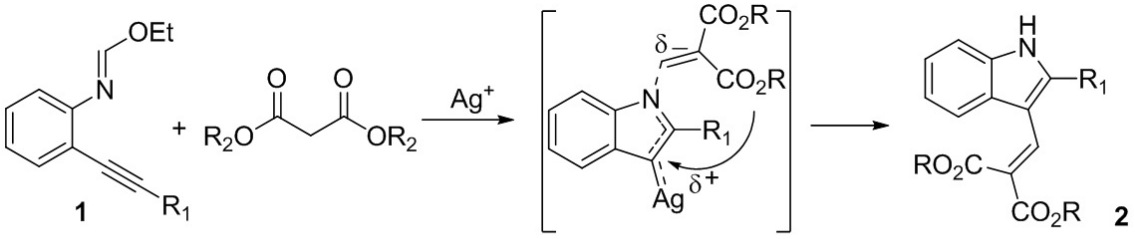
Transition metal-catalyzed Three-component Reactions to 2,3-Substituted Indoles

박효승, 박나리, *정지선, 오창호

*한양대 화학과 *한양대 자연과학대학 화학과*

Heterocyclic compounds, particulary indoles, are of interest because they widely occur in nature as partial structures of alkaloids and having unique biological activities. Recently, we observed a highly unique behavior involving 1,3-alkenyl shift to silver-carbenes in silver-catalyzed-cyclization of ethyl N-(2-alkynyl)phenylformimidates (1) with malonates. In this presentation, we report more efficient three-component version concerning 1,3-alkenyl shift leading to 2,3-substituted indoles (2) with some catalysts screening.



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N-H insertion reaction of *o*- aziidoaniline : solid-phase synthesis of Quinoxaline library

김용진

대구가톨릭대 화학과

we recently discovered that o-nitroanilines and o-azidianilines served as excellent substrates in N-H insertion reactions with rhodium carbenoids derived from α-diazo-β-ketoesters. The resin-bound N-H insertion products were cyclized by the treatment of $SnCl_2$ or TPP followed by DDQ to yield the corresponding quinoxalines, which were then further derivatized by a diversity-building, Lewis acid mediated amidation reaction upon cleavage.

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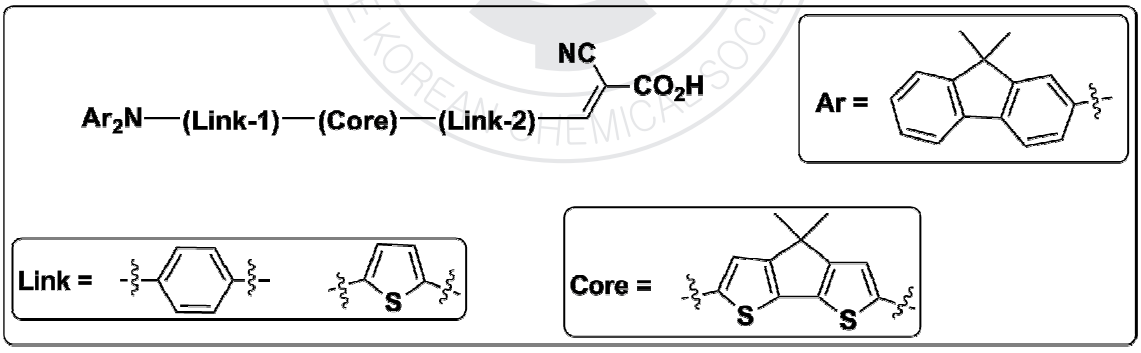
Synthesis of Organic Dyes with 4,4-Dimehtyl-4H-cyclopenta[2,1-b:3,4-b'] dithiophene Core and Structures in Dye-Sensitized Solar Cells

이형근, 이덕형

서강대 화학과

Recently, research interests on the renewable energy sources are increasing rapidly worldwide because the supply of fossil fuels will be limited eventually in the future. We describe herein the synthesis of six 4,4-Dimehtyl-4H-cyclopenta[2,1-b:3,4-b'] dithiophene Core-based organic molecules for Dye-sensitized Solar Cell(DSSC) and the energy efficiency of the solar cells derived from the dye.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-1**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Biological Evaluation of Novel Aminopyrrolidine Derivatives as CC Chemokine Receptor 2 (CCR2) Antagonists

임지웅, 나용호, 오유나, *조희영

*양지화학(주) 연구소 의약화학팀 *한국화학연구원 약리활성연구센터*

CC chemokine receptor 2 (CCR2) belongs to G-protein coupled receptor (GPCR) family, and the blocking of the interaction between natural ligand MCP-1 and CCR2 results in the variation of physiological activities including the abatement of inflammation. Thus, it has been suggested that antagonism mediated by monoclonal antibody or small molecule could be applied for the development of pharmaceutical candidates targeting on various inflammation-related diseases such as atherosclerosis, multiple sclerosis and several allergic diseases. We designed novel antagonistic structures toward CCR2 using GPCR homology modeling (CADD), and scanned some scaffolds through hCCR2b protein binding inhibitory activity together with functional assays including the chemotaxis and calcium flux inhibitions. After the SAR of hundreds of in-house synthetic compounds, N-benzoylpiperazinylethyl-5-aminopyrrolidine derivatives were found to show good potency in CCR2 antagonism. The results of subsequent in vitro assays and physical property tests demonstrated the usefulness of these compounds as drug candidates. Recent results from the preliminary study of anti-asthmatic efficacy (OVA-induced mouse model, inhaled administration) indicated that YJC-10450, one of our CCR2 antagonists, have an activity comparable to budesonide.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-2**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Biosensor System of Label-Free Protein Based on Polydiacetylene Liposomes

이혜원, 최혜, 최준식

충남대 생화학과

Protein delivery has been actively studied last two decades. However, effective detection systems have various limitations caused by labeling techniques and sensitivities. In this study, we synthesized nitrilotriacetic acid(NTA) to polydiacetylene(PDA) lipid using simple organic synthesis method and tried to protein detection and delivery by nickel-chelation.Liposomes based on PDA could be constructed upon polymerization via ultraviolet irradiation by 1,4-addition with alternating ene-yne groups in a row. The polymerized liposomes have visible color transition through various environmental pertubations such as pH, heat, ligand-receptor interaction and then detected label-free fluorescence. PDA has been studying as biological sensor systems because it makes easy to detecting using simple equipments.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-3**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Drug Discovery for Rheumatoid Arthritis by Inhibition of NF-kappaB Activation through IKK-2

김소라, *추현아

*고려대 화학과 *KIST 생체과학연구부*

Nuclear transcription factor NF-kappaB is responsible for the transcription of pro-inflammatory cytokines such as tumor necrosis factor alpha (TNF-alpha) and interleukin 6 (IL-6). Elevated levels of pro-inflammatory cytokines play an important role in the pathogenesis of inflammatory disorders such as rheumatoid arthritis (RA). Activation of NF-kappaB is mediated by activation of two kinases, IKK-1 and IKK-2, but IKK-2 is more critical than IKK-1 in activating the NF-kappaB pathway for inflammatory responses. Thus, IKK-2 is a good target for treatment of rheumatoid arthritis. Based on the known IKK-2 inhibitors, aminopyrimidine derivatives was designed, synthesized and biologically evaluated against IKK-2. The synthesis and biological activity will be discussed in detail.

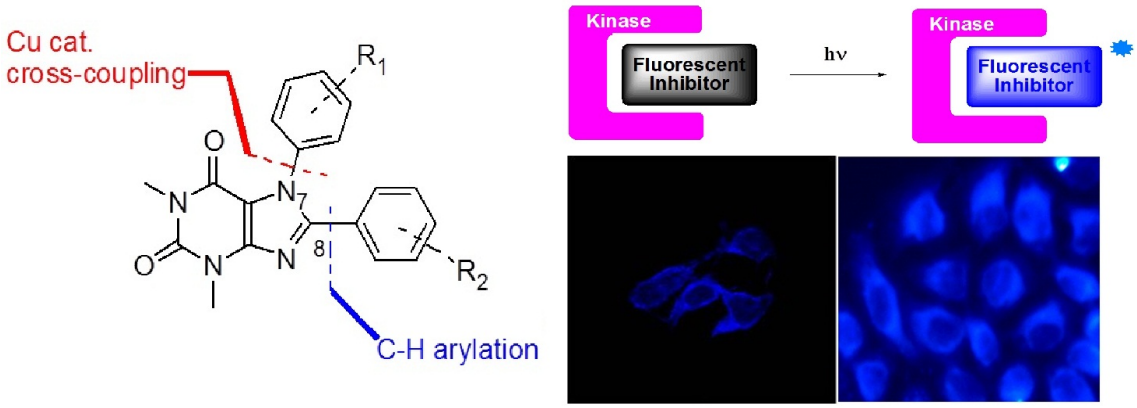
일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-4**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Phosphoinositide 3-Kinase Inhibitors that double as Intracellular Fluorescent Probes

김동희, *전휘석, **홍승우

*KAIST 화학과 *서울대 화학부 **KAIST 화학과*

An understanding of the intracellular drug distribution and fate in biological system is invaluable, since it can provide information whether drug reaches its desired target and a biological rationale for the design of new therapeutics with improved properties.An efficient and versatile synthetic approach for the preparation of highly substituted xanthine derivatives has been developed by a combination of direct N7- and C8-arylation. The xanthine core is structurally similar to ATP to fit into ATP binding site, while H-bonding of R1 and R2 moiety with S774 and K802 can increase binding affinity. This xanthine core skeleton can accommodate various emission maxima and quantum yield simply by changing substituents at the R1 and R2 positions, having different electronic properties. Herein, we report cell-permeable fluorescent PI3K inhibitors in which some part of the fluorophores were engineered to be pharmacophores binding to PI3K, and describe the monitoring of their distribution in cells.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-5**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Cu(II) Cyclen cleavage agent with BTA-derivative

정근홍, 정우영, 계영식, 김동욱, *김한일, *박두한

*육군사관학교학교 화학과 *삼육대 화학과*

Islet amyloid polypeptide, an oligopeptide with 37 amino acid residues, induces apoptotic cell-death in β-cell and causes an effect the development of Type 2 diabetes mellitus (T2DM). Cyclen cleavage agent with I-Box-derived binding group has been discovered as a potential therapeutic option for T2DM patients. Therefore, we synthesized Cu(II) cyclen cleavage agent with other binding group, BTA-derivative. The resulting activity and cleavage yield were evaluated after incubation with h-IAPP and identified that the activity of Cu(II) cyclen cleavage agent with BTA-derived binding group was higher than Cu(II) cyclen cleavage agent with I-Box-derived binding group.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-6**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Estimation of Prion Protein 106-126 amyloid aggregation rate and curcumin's aggregation inhibition rate

정근홍, 정우영, 계영식, 김동욱, *조경호, *배형은, *박두한

*육군사관학교학교 화학과 *삼육대 화학과*

Amyloid deposits are the hallmark of many neurodegenerative disorders including transmissible spongiform encephalopathies such as Creutzfeld-Jakob disease. The process of amyloid polymerization raises much interest because of the biomedical impact of this process. Several analytical methods have been developed to monitor amyloid aggregation rate. The determination of amyloid depositing is carried out by estimating fibril formation rate. Those techniques are not precise because it is not known that how many monomer proteins are composing the detected fibril. Here we succeeded in determining PrP 106-126 aggregation rate with exact figures for oligomers, succeeded in evaluating with exact figures curcumin's aggregation inhibition rate in vitro, and we showed that rotating during incubation does not influence on aggregation rate.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-7**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

방광암 특이적 펩타이드를 이용한 섬유선종의 진단

하영수, *곽원정, *유정수

*경북대 의과학과 *경북대 의과대학 분자의학교실*

대부분의 암은 몇 몇의 수용기를 과발현 하는 것으로 알려져 있다. 그리고 이러한 수용기를 표적으로 하는 작은 펩타이드를 이용한 종양의 진단과 치료가 지난 십여년간 이루어져 왔다. 여기에서 우리는 방광암 특이적 펩타이드로 섬유선종을 선명하게 영상화할 수 있다는 것을 보고하고자 한다. 9 개의 아미노산으로 구성된 방광암 특이적 펩타이드(BP)는 파지 디스플레이 방법으로 선발하고 스탠다드 펩타이드 합성법으로 합성하였다. 그리고 방사성요오드 표지화합물을 위해 아미노말단에 타이로신기를 연결하였다. 이를 Y-BP 라고 명명하였고 Y-BP 의 방사성요오드 표지는 Iodogen 으로 코팅된 튜브를 이용하였다. 동물모델은 쥐에 BBN(N-butyl-N-(4-hydroxybutyl)nitrosamine)을 처리하여 젖샘 부분에 암이 발생하도록 8 주동안 BBN 처리를 한 다음 실험에 적절한 암의 크기가 될 때까지 키워 사용하였다. 암 모델은 [^{18}F]FDG 와 방사성요오드 표지된 Y-BP([^{124}I]Y-BP)를 사용하여 microPET 영상을 얻었다. 또한 암을 절제하여 면역염색 실험을 실시하였다. 방사성요오드 표지된 [^{124}I]Y-BP 는 HPLC 로 정제하여 90% 이상의 방사화학적 순도로 분리하였다. 암은 [^{18}F]FDG 로 이미징 하였을 때 종양 부분의 몇 몇 병소부위에 머무는 것을 확인하였다. 하지만 [^{124}I]Y-BP 를 이용하여 주사 후 5 시간 뒤에 이미징 하였을 때 아주 명확하게 암에 Y-BP 가 머무는 이미지를 얻을 수 있었다. 그리고 암에서 3 일 동안 Y-BP 의 섭취를 관찰할 수 있었다. 이러한 암은 유선에서 유래된 섬유선종과 같은 조직학적 분석결과를 보였다. 방광암 특이적 펩타이드는 섬유선종을 포함한 다른 여러 종양을 탐지하기 위한 새로운 방사성 탐침자로서 큰 잠재력을 보여주었다.

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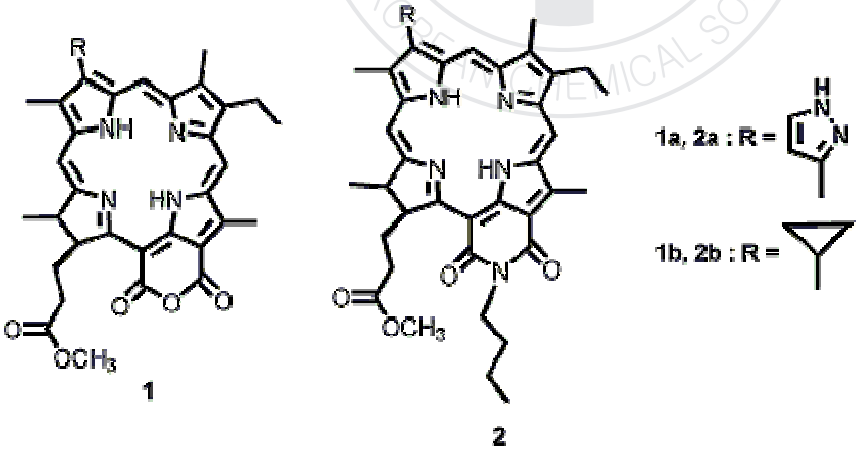
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and photodynamic activities of pyrazolyl and cyclopropyl chlorin derivatives

윤일, *박호성, *심영기

*인제대 PDT 연구소 *인제대 나노공학부*

The synthesis of new pyrazolyl and cyclopropyl chlorin derivatives is described. The new compounds were characterized by NMR, UV-vis spectroscopy and Mass spectrometry. The UV-vis spectra showed long wavelength absorption of ranges 692−708 nm (λmax). The chlorin derivatives were evaluated their photodynamic effects with A549 cells by WST-1 assay. The photodynamic activities showed high photocytotoxicity and low cytotoxicity in the dark.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-9**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

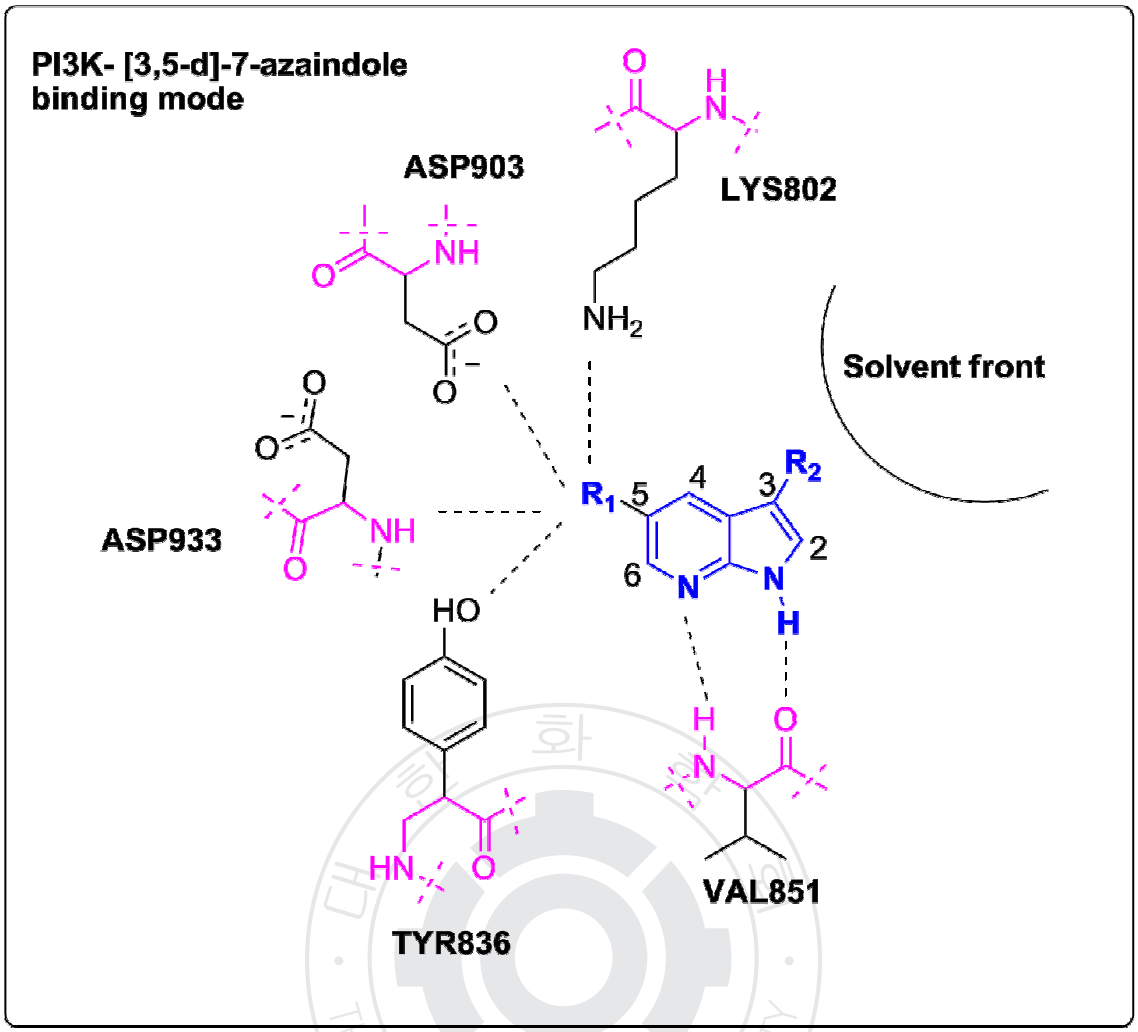
Discovery of Potent Azaindole-based PI3K Inhibitors: Apoptotic and Antiangiogenic Effect on Cancer Cells

홍승희, 홍승우

KAIST 화학과

Phosphatidylinositol-3-kinase(PI3K)is an important target in cancer due to the deregulation of the PI3K/AKT signaling pathway in many tumors. In this study, we identified [3,5-d]-7-azaindole as PI3K inhibitors, which were designed based on molecular modeling of compounds bound to PI3K. SAR(Structure-Activity-Relationship)studies, by varying 3,5- positions, lead to the discovery of a series of potent PI3K inhibitors. As a result of in vitro biological test, azaindole compounds exhibited good potencies over PI3K and anti-proliferative activity.

KOREAN CHEMICAL SOCIETY


PI3K- [3,5-d]-7-azaindole
binding mode
ASP903
LYS802
Solvent front
ASP933
TYR836
VAL851
R1
R2
NH2
HO
NH
HN
H
N
O

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-10**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and 11beta hydroxysteroid dehydrogenase 1 inhibition of thiazolidine derivatives with an adamantyl group

이재홍, *복주한, **강승규, ***김기영, ****이상달, *****배명애, ******안진희

*고려대 화학과 *한국화학연구원 대사증후군센터 **한국화학연구원 대사증후군치료제연구센터 ***한국화학연구원 신약연구단 ****한국화학연구원 분자약리연구팀 *****한국화학연구원 신약플랫폼기술팀 ******한국화학연구원 대사성질환연구팀*

A new series of thiazolidine derivatives with an adamantyl group was synthesized and evaluated for their ability to inhibit 11beta-hydroxysteroid dehydrogenase 1 (11beta-HSD1). Our initial compound 5a showed a weak inhibitory activity. Significant improvements in potency were achieved by substituent modification. The most potent compound 8g (E) showed good in vitro inhibitory activity toward human 11beta-HSD1, selectivity toward 11beta-HSD2, metabolic stability, pharmacokinetic and safety profile. Furthermore, this compound significantly inhibited 11beta-HSD1 activity in rat and monkey models, and showed improved glycemic control in KKAy mice.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Solid-phase Synthesis of Novel Pyrazole Derivatives via Thiourea Linker on BAL Resin

윤도경, 김미선, 공영대

동국대 화학과

Solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of an ongoing drug discovery program, we have been exploring the potential of resin-bound pyrazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of pyrazole based library through resin-bound thiurea linker on BAL resin. During about the past decade 1,3,4,5-substituted pyrazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. 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 upon cleavage from the resins.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-12**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 2-Alkylamino substituted-1H-benzo[d]imidazole Derivatives via Thio-carbarzate Linker on Merrifield Resin

김미선, 김지혜, 이재민, 공영대

동국대 화학과

Synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Therefore, we have been exploring the potential of resin-bound benzo[d]imidazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a unique parallel synthetic method for combinatorial generation of 2-alkylamino substituted-1H-benzo[d]imidazole derivatives via thio-carbazate linker. The 2-alkylamino substituted-1H-benzo[d]imidazole derivatives have attracted much attention for their interesting various biological activity such as COX-2, 5-LO, and various receptors. The final compounds were obtained in good yields and high purities upon cleavage from the Merrifield resin.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 2-Alkylamino substituted-1H-benzo[d]imidazole Derivatives via Thiourea Linker on BAL Resin

장소영, 배미선, 공영대

동국대 화학과

Synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Therefore, we have been exploring the potential of resin-bound benzo[d]imidazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of benzo[d]imidazole based library through resin-bound BAL linker. During about the past decade 2-amido/amine substituted benzo[d]imidazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-14**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 2-Amido/amine substituted benzo[d]oxazole Derivatives via Thiourea Linker on BAL Resin

정세린, 배미선, 공영대

동국대 화학과

Synthesis has become an extremely powerful technique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Therefore, we have been exploring the potential of resin-bound 2-amido/amine substituted benzo[d]oxazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Especially, we were interested in construction the variously substituted 2-amido/amine substituted benzo[d]oxazole library because of their broad biological activities. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of 2-amido/amine substituted benzo[d]oxazole library through resin-bound benzo[d]oxazole via thiourea linker on BAL resin.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표코드: **MEDI.P-15**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A Novel Phenylimidazo[1,2-a]pyridine Core Skeleton and Pharmacophore Model as Hypoxia-Inducible Factor Inhibitors

배미선, 공영대, *강남숙

*동국대 화학과 *한국화학연구원 신약플랫폼기술팀 분자설계*

The importance of HIF-1α in the mediation of normal and pathological processes has motivated considerable efforts to identify HIF-1α inhibitors. Although a wealth of inhibitory compounds are available, synthesizing HIF-1α inhibitors with a novel small-molecule core skeleton fitting individual HIF-1α has proven to be a challenge. Here, we report initial evidence showing that compounds with a phenylimidazo[1,2-a]pyridine core skeleton are selective HIF-1α inhibitors, and have potential as anticancer agents in treatment. The aim of this study was to investigate the biochemical properties of HIF-1α and to identify new core skeleton inhibitors of HIF-1α. To identify small-molecule inhibitors of HIF-1α, we screened 1,200 compounds using the HRE/SW480 stable cell line containing HRE-luc[pHTS-9XHRE-Luc].These 1,200 compounds represent structurally diverse and druggable 20,000-member heterocyclic compound libraries, including imidazole, benzopyrans, oxazoles, thiazoles, thiadiazoles, and pyridines.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 2-Alkylamino substituted-1H-benzo[d]thiazole Derivatives via Thiourea Linker on BAL Resin

심주용, 김지혜, 공영대

동국대 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. And solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound benzo[d]thiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of benzo[d]thiazole based library through resin-bound BAL linker. The 2-alkylamino substituted-1H-benzo[d]thiazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. The final compounds were obtained in good yields and high purities upon cleavage from the resins

일시: 2010년 10월 14~15일(목~금) 2일간
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Solid-phase Synthesis of Oxadiazole and Thiadiazole Derivatives via Thiourea Linker on BAL Resin

양승주, 김미선, 공영대

동국대 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. And solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound oxadiazole and thiadiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of oxadiazole and thiadiazole through resin-bound thiourea linker on BAL resin. The 2-alkylamino oxadiazole and thiadiazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표종류: 포스터, 발표일시: 금 10:30~12:30

Role of ^{99m}Tc-DMSA in Assessing Kidneys Repair Capacity

TAKELE, *곽원정, *유정수

*경북대 의과학과 *경북대 의과대학 분자의학교실*

Quantitative ^{99m}Tc-DMSA renal uptake was studied in different renal ischemia-reperfusion (I/R) mice models for the assessment of renal repair capacity. Mice models of nephrectomy, uni-lateral and bi-lateral I/R together with sham operated mice were established. At 1 hr, 1 day, 3 days, 1 week, 2 weeks and 3 weeks after I/R ,^{99m}Tc-DMSA (27.7 ± 1.3 MBq) was injected via tail vein and after 3 hrs p.i, the mice were scanned for 30min with phinhole equipped gamma camera. Higher uptake of DMSA (15- 80%) was measured in normal left kidneys of I/R model followed by nepherctomized kidneys as a result of compensatory physiological hyper-functional DMSA uptake. The patterns of reduced DMSA uptake in the right and left kidneys of the bi-I/R models closely paralleled. Comparing the restoration capacities of the affected kidneys of uni-lateral and bi-lateral I/R models, higher repair capacity was observed in the latter models. The normal kidney may interrupt the restoration of damaged kidney. In summary, considering the inherent drawbacks of histopathological and immunostaing techniques for the assessment of renal functions, we evaluated DMSA scan and showed its potential as a promising noninvasive method for evaluation of function of renal tubular cells. Moreover, our experiments also indicate that mice with bi-I/R had higher repair capacity than those with uni-I/R. This suggests that patients with bi-lateral kidney problems may recover faster than those patients with uni-lateral kidney problems, which is contrary to what usually was anticipated

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Cytotoxic Activity of Clotrimazole Derivatives

정순재, *김인종, *박정훈, **김상욱, *허민구, *양승대, 유국현

*동국대 화학과 *한국원자력연구원 방사선생명공학연구부 **동국대 나노소재화학화*

The clotrimazole [1-{(2-chlorophenyl)-diphenylmethyl}-1*H*-imidazole] has been reported to inhibit the proliferation of vascular endothelial cells and act as an anti-VEGF (vascular endothelial growth factor) drug in vitro. The clotrimazole is also shown to inhibit the angiogenesis in an animal model. In our previous attempt, we synthesized *N*-[^{18}F]fluoroalkylclotrimazolium as a novel potential PET radiotracer. In present study includes, we synthesis of *N*-hydroxyalkylclotrimazolium for the investigation of the anticancer effect. The clotrimazole is treated with tosyloxyalkyl acetate to give *N*-acetoxyalkylclotrimazolium in 30% yield. The hydrolysis of *N*-acetoxyalkylclotrimazolium in 1 N HCl gave the *N*-hydroxyalkylclotrimazolium in 50% yield. We tested the cytotoxicity of *N*-fluoroalkylclotrimazolium and *N*-hydroxyalkylclotrimazolium using a RAW 264.7 macropharge cell by quantitative RT-PCR analysis.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Biological Evaluation of new Quinuclidine derivatives as Potential Therapeutic Agents for Alzheimer's Disease

최연희, *김영습, **배애님, **이재균, *최기항, **조용서, **민선준

*상명대 화학과 *고려대 화학과 **KIST 생체과학연구본부*

Alzheimer's disease (AD) is an age-related, chronic neurodegenerative disorder occurring in middle or late life. The disease is characterized by a progressive dementia, which is associated with both severe disabilities in performing the activities of everyday life and a reduced life expectancy after onset of the disease. The disease is estimated to currently affect three to four million people in the United States, and its prevalence is increasing as a greater proportion of the population reaches a longer life expectancy.Although the etiology of AD is unknown, histopathological hallmarks such as amyloid β (Aβ) deposits, τ-protein aggregation, oxidative stress, and low levels of acetylcholine (ACh) have been characterized.Recent study reported that Dimebon, clinically used as an antihistaminic drug in Russia since 1983, exhibited neuroprotective effects along with cognition-enhancing effects in clinical trials. It appears to operate through multiple mechanisms of action including inhibition of Aβ aggregation and blocking mitochondrial permeability transition pores (MPTP). Therefore, inhibition of mPTP in the brain may provide a new avenue for treatment of AD.We here report synthesis and biological evaluation of quinuclidine derivatives as potential MPTP blockers.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Improvement of pharmacological profile of mibefradil, a selective T-type calcium channel blocker: Synthesis and biological evaluation of dihydrobenzofuran analogues derived from mibefradil

구수진, *신선미, **한소엽, ***배애님, ***이재균, ***민선준, ***조용서

*이화여대 화학,나노과학부 *이화여대 화학 나노 과학과 **이화여대 화학나노과학과, 촉매반응·합성연구센터 ***KIST 생체과학연구본부*

Voltage-gated Ca2+ channels play an important role in the control of intracelluar process in cardiac, vascular and neuronal tissues. They are divide into two classes, high-voltage-activated (HVA) calcium channel and low-voltage-activated (LVA) or transient (T-type) calcium channel. T-type Ca2+ channels are encoded by a family of related genes, Cav3.1 (α1G), Cav3.2 (α1H), and Cav3.3 (α1I). It has been reported that the α1G and α1I subtypes are primarily expressed in CNS neurons and peripheral tissues. Therefore, they may have potential for the treatment of neurological disorders such as epilepsy and neuropathic pain. Mibefradil was launched as the first selective T-type calcium channel blocker, demonstrating a high antihypertensive activity. However, it was withdrawn from the market in 1998 because of potentially harmful interactions with other medications (Terfenadine, Astemizole, Cisapride), which are caused by CYP enzymes, expecially, CYP3A4 isozyme. The metabolic study of mibefradil turned out that hydroxylation at the benzylic carbon of the tetrahydronaphtyl ring is the most important metabolic process in microsomes. In this regard, we have synthesized several mibefradil analogues having oxygen atom at the bezylic position of tetrahydronaphthalene by replacing methylene carbon with oxygen to prevent metabolic oxidation. Herein, we will present the channel blocking activities of these compounds against T-type calcium channels, their metabolic stabilities in human hepatic microsomes, and their CYP inhibitions.

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Synthesis and Binding affinities of 1,2,3-triazolyl-ethylpiperazine library as Dopamine receptor

곽주명, *서용완, 최정화, 고훈영, 이해황

*인하대 화학과 *인하대 자연과학대학 화학과*

The 1,2,3-triazole heterocyclic structure is well known as an one of the potential key molecular structure for the biologically meaningful drug design.Recently, the synthetic study on 1,2,3-triazole heterocyclic structure is a main concern in the field of click chemistry. In this study, 1,2,3-triazole-ethyl-piperazine was synthesized under echo-friendly reaction condition by using of microwave synthesizer. Constructed fifty two compounds were screened against dopamine receptor in vitro.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
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Construction and Binding affinity of n-Butyl Pyrazole Library as Antagonist of D4 receptor

서용완, *Kamalkishor, *고훈영

*인하대 자연과학대학 화학과 *인하대 화학과*

The malfunction of central nervous system is well known to be the cause of mental disorder for a long time. Recently, it is well known that dopamine D4 receptors in mental disorder such as schizophrenia or attention deficit hyperactivity disorder [ADHD] had to be involved. In this study, the n-butylpyrazole heterocyclic library coupled with the phenyl piperazine derivatives were designed as the promising candidate molecular structure on the selective dopamine D4 receptor antagonist. From the well established synthetic pathway, a library of 52 compounds was synthesized and evaluated for their biological activity in vitro. The screening results of a few selected compounds on the dopamine D4 receptor were shown the excellent IC50 value under 10 nM scales.

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Isolation and identification of rutin from *Allium Mongolicum*

tuyagerel, *홍유진, 이범종

*인제대 화학과 *인제대 바이오헬스소재학과*

Plants of the genus *Allium* have been recognized as rich sources of secondary metabolites. *Allium Mongolicum* is an endemic native plant in Mongolia. In tradition of Mongolia, this plant has been used for food such as onion. There is no information about the isolation of any bioactive secondary metabolites from this plant. The purpose of our study is to isolate bioactive compounds from *Allium Mongolicum*. We isolated rutin from ethyl acetate fraction of *Allium Mongolicum*, which shows anti-oxidant activity. Rutin (rutoside, quercetin-3-rhamnosyl glucoside and sophorin) is a member of bioflavonoids. Rutin has anti-oxidant, anti-inflammatory, antiallergenic, antiviral, and anti-carcinogenic properties. We analysed the anti-oxidant activity of the rutin by some in-vitro assay methods. The structure of the rutin has been elucidated by combined spectroscopic methods including ^{13}C and ^{1}H-NMR, IR, UV-Vis and elemental analysis.

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

A concise synthesis of stilbene analogues for Atherosclerotic Cardiovascular Disease

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 such as antioxidant, cardiovascular and anticancer. Several study proved reduction of reactive oxygen species could be an effective therapeutic intervention in atherosclerosis. Based on the above considerations, we investigated a convenient synthesis and biological properties of new derivatives of trans-stilbene. All analogues were evaluated for free radical-scavenging activity. Most of the trans-stilbene derivatives showed 2–3 times more radical-scavenging activity than resveratrol. This result suggests that the prepared stilbene analogues exhibited a possibility for cardiovascular agent.

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Synthesis and Biological Evaluation of Deoxoartemisinin Trimers for Anti-Angiogenesis

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, oral and renal cancer cell lines. We synthesized trimers of deoxoartemisinin and evaluated its angiogenesis activity. In this study, the trimers of deoxoartemisinin showed the potent anti-angiogenesis inhibition effect (% inhibition = 40~64 %), even better than fumagiline and (-)-thalidomide.

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One Pot Synthesis of 5-[^{18}F]fluoroisoquinolin-1-ol

김희정, 김동연, 이지은, *김인종, *박정훈, **김상욱, *허민구, *양승대, 유국현

*동국대 화학과 *한국원자력연구원 방사선생명공학연구부 **동국대 나노소재화학화*

Pharmacological inhibition of poly(ADP-ribose)polymerase(PARP) has demonstrated significant anti-tumor effect in several cancers such as glioma, melanoma and breast cancer etc. The compound 1,5-isoquinolinediol was found to be an attractive chemotherapeutic agent for PARP. PARP inhibitors (i.e. 1,5-isoquinolinediol) can be considered useful ingredients for the treatment of cancers. The target compound, 5-[^{18}F]fluoroisoquinolin-1-ol in prepared by one-pot Balz-Schiemann reaction. The compound was synthesized to investigate its potential for a cancer imaging agent for PET. The Balz-Schiemann reaction allowed the introduction of fluoride in to the aromatic compounds but in the radiofluorination, it has a critical limit due to low specific activity because $^{19}F^-$ and [^{18}F]F^- coexisted for the Balz-Schiemann reaction. We tested one-pot reaction to solve this problem. The separation and purification of 5-[^{18}F]Fluoroisoquinolin-1-ol was done by HPLC (stationary phase: phenomenex SYNERGI 150×4.6 ㎜ 4 ㎛ column; mobile phase: H_2O/EtOH(75/25) 1mL/min; Rt: 15min). The radiochemical yield found to be ~10% and radiochemical purity was observed above 95%. F-18 labeled isoquinoilne derivative with high specific activity (≥60GBq/μmol) has been synthesized via one-pot Balz-Schiemann reaction.

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A novel micelle-encapsulated platinum(II) anticancer agent

Vithal Jadhav, 전용주, *손연수

*이화여대 화학·나노과학과 *씨앤팜 부설연구소*

A hydrophobic and water-insoluble platinum(II) compound, cis-$(cha)_2Pt(NO_3)_2$ was encapsulated by macromolecular micelles self-assembled from an amphiphilic cyclotriphosphazene $[NP(MPEG750)(GlyPheLeu)_2Et]_3$ (CP750). The micelle-encapsulated platinum(II) compound exhibited outstanding pharmacokinetics in rats by showing long blood circulation and much larger systemic exposure (AUC = 43.5 μg•h/ml) compared with the free carboplatin (AUC = 4.32 μg•h/ml). Biodistribution study using male Sprague-Dawley rats has shown excellent tumor selectivity of the micellar platinum(II) compound with the tumor to tissue ratios of 4.03 at 2 h post injection and 4.67 at 24 h post injection. Furthermore, the micellar platinum(II) compound exhibited more than 6 times higher cellular uptake in human cervical (HeLa) and lung (A5490) tumor cells compared with the free platinum compound. Also it is surprising that the micellar platinum(II) compound displayed specifically high cytotoxicity against the stomach tumor cells (SNU638), which are one of the least responsive to chemotherapeutic agents currently in clinical use. Thus the platinum compound encapsulated by cyclotriphosphazene micelles is a promising candidate for clinical studies.

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A Tumor-selective Prodrug of Polyphosphazene-Paclitaxel Conjugate

전용주, *손연수

*이화여대 화학·나노과학과 *씨앤팜 부설연구소*

Paclitaxel is one of the most important antitumor agents currently in clinical use, since it exhibits effective antitumor activity against various cancers, such as breast, ovarian, and non-small cell lung cancers. However, its clinical applications are limited due to its extremely low water solubility (< 1 μg/ml) and serious side effects including hypersensitivity and neurotoxicity attributed to its formulating agent, Cremophore EL. Among many different approaches to overcome such problems, intensive studies on paclitaxel-polymer conjugates have been made for last decades. In this study, a novel water-soluble and biodegradable polyphosphazene-2`-succinylpaclitaxel(SPTX) conjugate was prepared by reacting 2'-succinylpaclitaxel(SPTX) with polyphosphazenes bearing equimolar glycyl-L-lysine and methoxy poly(ethylene glycol) as side groups. The resultant macromolecular conjugate was found to self-assemble in aqueous solution to form a stable micelle with a mean hydrodynamic diameter of 9-13 nm and a low critical micelle concentration of about 40 mg/L. The biodistribution study of the Cy5.5-labelled polyphosphazene-2`-SPTX conjugate using NIR-fluorescence images has shown outstanding tumor selectivity.

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Synthesis and biological evaluation of heterocyclic compounds as Nitric Oxide Synthases (NOSs) inhibitors

표정인, 김관수, *정찬성

*연세대 화학과 *KIST 케모인포매틱스연구단*

Nitric Oxide (NO) is enzymatically produced from terminal nitrogen atom of L-arginine, dioxygen (O_2) dependent oxidation and cofactor (BH_4, FMN, FAD, NADPH, heme) catalyzed by Nitric Oxide Synthases (NOSs). It is classified three isoforms through the physical functions or pathological process for smooth muscle (endothelial NOS, eNOS), neuronal signaling (neuronal NOS, nNOS) and immune response (inducible or inflammatory NOS, iNOS). The overproduction of metabolite NO has been a factor of various diseases such as cardiovascular, gastrointestinal, genitourinary, respiratory and nervous systems. In our study, new potent and selective inhibitors of NOSs were prepared by using electrophilic aromatic substitution of the pyrimidine structure under Vilsmeier-Haack formylation.

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Synthesis and evaluation of heteroaryl substituted 5,6-Dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives as MCH receptor 1 antagonist

임채조, *이은경, 김지영, 김낙정, 이규양, **송석진

*한국화학연구원 대사증후군치료제연구센터 *과학기술연합대학원대 의약및 약품화학 **유유제약 중앙연구소*

The melanin-concentrating hormone receptor (MCH-R1) as a cyclic 19-amino acid neuropeptide is one of the most promising targets in treatment of obesity. In continuation of our efforts to search for new scaffolds of MCH-R1 antagonists, we have identified a series of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives and examined the effect of various heteroaryl group at 2-position of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one to the MCH R1 binding activity. As a result, we have found that several compounds exhibited high MCH-R1 binding affinity in vitro assay. The details of synthesis and binding affinity will be discussed.

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발표코드: **MEDI.P-32**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and evaluation of benzyl and alkyl substituted 5,6-Dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives as MCH receptor 1 antagonist

임채조, 서무영, 왕수미, 김낙정, 이규양, *송석진

*한국화학연구원 대사증후군치료제연구센터 *유유제약 중앙연구소*

Antagonists of the melanin-concentrating hormone receptor (MCH-R1) have great potential utility for the treatment of obesity. Previously we have identified a series of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives as new MCH R1 scaffold. As part of our efforts on the optimization of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one, we investigated the variation of benzyl and alkyl group at 2-position on 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one. From the results of SAR study, we have found that several compounds showed excellent MCH-R1 binding affinity in vitro assay. The detailed results of structure-activity relationships (SAR) will be presented.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-33**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and biological evaluation of oxazoles as tubulin polymerization inhibitors

노은선, *최경일, *남길수, 태진성

*연세대 화학과 *KIST 생체과학연구본부*

In recent years, development of anticancer drug is a major topic of medicinal chemistry. The biological importance of microtubules in mitosis and cell division makes them interesting as cancer target. The tubulin polymerization inhibitor can act as anti-mitosis by inhibiting G_2/M phase in cancer cell, and also is known as vascular disrupting agent for its selectivity in blocking proliferation of vascular cell near cancer cell. Small molecules such as colchicin, ABT-751 and AS-1404 are attractive as inhibitors of tubulin polymerization. In this presentation, we discuss the synthesis of a new class of oxazole scaffold having electron-donating and electron-withdrawing substituents, and their biological evauation for antiproliferative activity and tubulin polymerization inhibitory activity. The most promising compound of this series showed good cancer cytotoxicity in nanomolar concentrations and potent inhibitory activity of tubulin polymerization in micromolar range.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-34**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and biological evaluation of aryl oxazole derivatives as tublin polymerization inhibitor

최민정, 고수영, *조용서, *배애님

*이화여대 화학과 *KIST 생체과학연구본부*

Cancer represents one of the most threatening disease of mankind. Within the last decade, the treatment of cancer has been studied for understanding of malignant cell growth and regulation of the cell cycle machinery. Tubulin is one of the main element in mitotic period and plays an important role in cell division. Dual effects of tubulin interfering agents are to lead an apoptosis of tumor cells throughout interrupting cell division and to induce vascular damage within tumors. With this advantage, the development of tubulin interacting agents has been studied on cancer therapeutic and interruption of tumor vascularization. In this study, we designed and synthesized new small molecules having oxazole core as potential tubulin inhibitors. They were biologically evaluated by cell-based anticancer assay and tubulin polymerization assay. The compounds were tested on HUVEC vascular disruption assay. The design, synthesis and biological evaluation of the synthesized compounds will be presented.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and anti-cancer activity of 3,5-diaminoindazole derivatives

김진아, *박종원, 이진호

*계명대 화학과 *대구경북과학기술원 나노바이오연구부*

Protein kinases are involved in signaling pathway of both normal and cancerous cells. These enzymes play a major role in biological processes as control of cell growth, metabolism, differentiation and apoptosis. Protein kinases are become a hot target to develop small molecules as potential inhibitor that can alleviate diseases caused due to abnormalities in signaling pathways. Our previous study in development of novel anti-cancer agents led to the identification 3,5-diaminoindazoles as potent CDK inhibitors. The substitution at position 5 of indazole by 1-λ^6-isothiazolidine-1,1-dione was found to increase enzyme inhibitory activity and growth inhibition of cancer cell lines. Drawbacks of this functional group are poor solubility and low oral absorption. Searching for new functional groups with improved physical properties was performed. After 5-fluoropyrimidine derivatives was found to show very potent anti-proliferative effect, further modification of the substituent at 3 and 5 positions of indazole were performed. Cell growth inhibitory effect and aqueous solubility of synthesized compounds were studied.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Specific detection of c-reactive protein by molecularly imprinted monolayer based on click chemistry

박종원, 김은주, 김현철, 정상원

대구경북과학기술원 나노바이오연구부

We report two-dimensional (2D) molecular imprinting of C-reactive protein (CRP) on a gold surface based on click chemistry and the binding characteristics of the resulting molecularly imprinted monolayer. CRP is one of the pentraxin proteins and has five calcium-dependent binding sites for phosphocholine. 11-Azidoundecane-1-thiol (azido-thiol) and 12-propargyloxydodecylphosphorylcholine (propargyl PC) were synthesized as monomers for click reaction, and five molecules of propargyl PC were reacted with one CRP molecule. The CRP-propargyl PC complex was allowed to react to azido-thiol modified gold surface, preserving the ligand arrangement of pentameric CRP-specific binding sites. Finally, the bound CRP was dissociated by elution buffer containing 10 mM EDTA and then the rebound capability of CRP-imprinted monolayer was determined by surface plasmon resonance (SPR) measurement. The binding constant of imprinted monolayer was $1.5X10^8$ M^{-1}, calculated by Langmuir isothermal equation (R^2 >0.99). The human serum proteins did not showed any inhibition effect to CRP binding, which showed increased selectivity for CRP in imprinted monolayer. In conclusion, we propose that the CRP imprinted monolayer could be used as a synthetic antibody sensor for detection of CRP.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-37**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

In silico toxicity screening for cardiac system

박지현, 이성광

한남대 화학과

The hERG(human ether-a-go-go related gene) potassium channel is a main factor for cardiac repolarization, and the blockade of this channel could induce arrhythmia and sudden death. Therefore, potential hERG blockers are now a primary concern in the drug discovery process, and lots of efforts are focused on the minimizing the undesirable side effect. IC50 data of 202 organic compounds in HEK (human embryonic kidney) cell was obtained from literatures. The external validation are carried out in experimental dataset of hERG inhibitors on the basis of CHO(Chinese hamster ovary) cell. Multiple linear regression(MLR), partial least square regression(PLS), and artificial neural network(ANN) were appled to model the inhibition of hERG. Genetic Algorithm (GA) combined with cross-validation procedure was used to select best subset descriptors for each learning algorithm.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Predicting the binding affinity of androgen receptor for diverse organic chemicals

전을혜, 이성광

한남대 화학과

146 natural, synthetic and environmental chemicals have potential to disrupt the endocrine system of human and wildlife. These chemicals, termed endocrine disrupting chemicals (EDCs), mimic or antagonize the functions of natural hormones. Androgens play an important role in the maintenance of the male phenotype. In this study, we have developed two-dimensional quantitative structure-activity relationship (2D-QSAR) models to examine the AR-ligand binding affinities. 2D-QSAR was designed on the basis of three methods, multiple linear regression (MLR), neural network (NN) and support vector machine (SVM). We used relative binding affinity to the androgen receptor (AR) as end point. These predictive models give light on the identification of potential androgenic endocrine disrupting compounds.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of plastoquinone marine natural products from a useful natural marine source

심진희, *오상태, *이석준

*관동대 의대연구실 *관동대 의과대학 기초과학교실*

There are various kinds of plastoquinone marine natural products in the family of Sargassaceae algae. Because those compounds show useful biological activity including antioxidant activity, insect growth inhibition, cytotoxicity, and so on, many researches have been undergoing on the novel drug discovery. However, the amount of marine natural products originated from marine sources is extremely small, and it is the main obstacles to obtain novel drug candidates. Recently, we have found a species of Sargassaceae algae that contains a useful starting material to be able to synthesize plastoquinone marine natural products. In this presentation, we will show an example to synthesize several plastoquinones which was discovered in 2008.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

The effect of EGCG on blood glucose level and the application of green tea on diabetes alleviation

노준호, 이진호

계명대 화학과

Type 2 Diabetes mellitus, accounts for more than 95% of all cases of diabetic patients in Korea, is known to have strong genetic tendency. In addition, the number of people with diabetes is increasing due to aging, urbanization, and increasing prevalence of obesity and physical inactivity. Green tea has been used in the development of drugs for diabetes based on the blood glucose level lowering effect. However, it was not effective in clinical trials so far. To understand the clinical results, the effects of green tea on glucose level were reexamined. Epicatechin gallate (ECG) and Epigallocatechin gallate (EGCG), the major catechin components of green tea, were confirmed to have a strong effect on the blood glucose level control as previously reported. However, it was found that the effect was time dependent. In gastrointestinal (GI) tract, EGCG inhibited the absorption of glucose into the circulation and provided low blood glucose level. However, once EGCG went into the circulation, it caused high blood glucose level by blocking the glucose uptake into tissues. Initially, we tried to find the ways which could selectively reduce the content of EGCG from green tea to compensate the dual effects. Later, based on the results, the method which could inhibit the absorption of the EGCG into the circulation while maintaining the role of green tea in the GI track was found. With the findings, green tea can be used as effective blood glucose level regulator.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

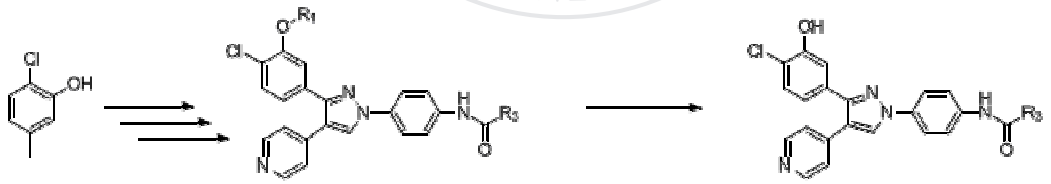
Synthesis and antiproliferative activites of 1-substituted-3-(4-chloro-5-methoxyphenyl)-4-pyridinylpyrazole and 1-substituted-3-(3-chloro-4-methoxyphenyl)-4-pyridinylpyrazole derivatives for melanoma cell

최원경, *박진헌, 최기항, **유경호, **조정혁, ***오창현

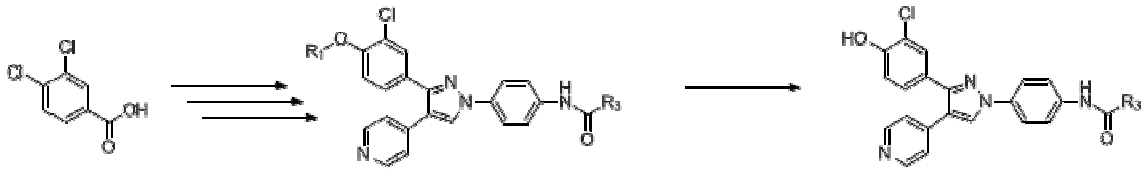
*고려대 화학과 *경희대 기초약학과 **KIST 생체과학연구본부 ***KIST 바이오소재연구센터*

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-(4-chloro-5-methoxyphenyl)-4-pyridinylpyrazole and 1-substituted-3-(3-chloro-4-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.

1-substituted-3-(4-chloro-5-methoxyphenyl)-4-pyridinylpyrazole scaffold



1-substituted-3-(3-chloro-4-methoxyphenyl)-4-pyridinylpyrazole scaffold



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-42**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Tautomerism of Small Molecules Studied with Activation Energies and pK_a Values by Quantum-Mechanical Calculations

이주연, 강남숙, *강영기

*한국화학연구원 신약플랫폼기술팀 분자설계 *충북대 화학과*

Tautomeric forms of molecules differ in shape, functional groups, and hydrogen-bonding pattern. Calculations of physical-chemical properties and molecular descriptors such as logP calculation, similarity index, and the ligand-protein interactions differ from one tautomeric state to the other. The interconversion between two tautomeric forms is quantitatively described by the equilibrium constant K_T, which is defined as the concentration ratio of the two tautomers in equilibrium. We used the activation energy, $\triangle G^{\ddagger}$ from one tautomeric state to the other, and their pK_a values to obtain K_T values of molecules, and all calculations are carried out using various Quantum-Mechanical (QM) methods. Here, we can propose an appreciate QM calculation for the prediction of tautomerism of small molecules.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of ^{68}Ga-labelled protoporphyrin dimethyl ester for tumor diagnosis

이은선, 박정훈, 김인종, *김상욱, 허민구, 양승대, **유국현

*한국원자력연구원 방사선생명공학연구부 *동국대 나노소재화학화 **동국대 화학과*

Ga-68 displays excellent decay properties with a half-life of $T_{1/2}$= 68 min and positron abundance of 89%. Ga-68 is easily obtained from ^{68}Ge/^{68}Ga generator without a cyclotron on site. Ga-68 is suitable for imaging tumors using positron emission tomography (PET). Due to accumulation of porphyrin derivatives on tumor cell, it's diagnosis becomes easy. Hence Ga-68 labelled to porphyrin as a novel potential PET radiotracer will be promising tumor imaging agent in cancer. In this study, we synthesized [^{68}Ga]Gallium-protoporphyrin dimethyl ester, for this purpose protoporphyrin dimethyl ester is chelated with [^{68}Ga]GaCl3$_3$ which is obtained from ^{68}Ge/^{68}Ga generator eluted with 0.1 N hydrochloric acid. In the solution of protoporphyrin dimethyl ester in acetonitrile was added [^{68}Ga]GaCl$_3$ in 0.1N hydrochloric acid over about one hour at 100℃. Finally [^{68}Ga]Gallium-protoporphyrin dimethyl ester was separated using HPLC. The radiochemical yield of [^{68}Ga]Ga-protoporphyrin dimethyl ester was found to be 18% respectively. [^{68}Ga]Ga-protoporphyrin dimethyl ester was carried out as a tumor imaging agent for PET. The biological evaluation is going on.

일시: 2010년 10월 14~15일(목~금) 2일간
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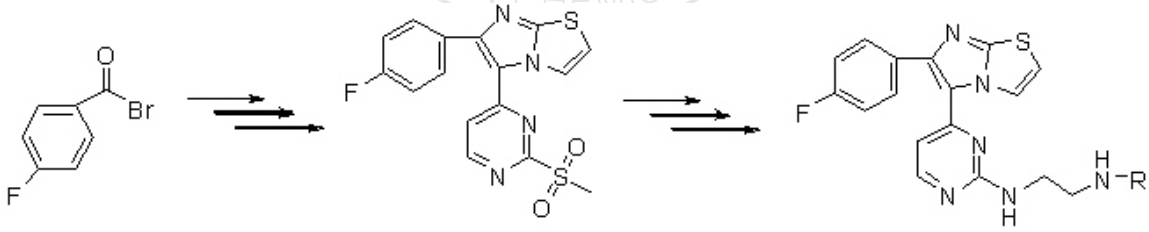
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of new 6-(4-fluorophenyl)-5-(substituted pyrimidin-4-yl)imidazo[2,1-b]thiazole derivatives and their antiproliferative activity against melanoma cell line

박진헌, *최원경, **이용섭, ***심태보, ***유경호, ***조정혁, ****오창현

*경희대 기초약학과 *고려대 화학과 **경희대 약학과 ***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 6-(4-fluorophenyl)-5-(substituted pyrimidin-4-yl)imidazo[2,1-b]thiazole derivatives is described. Their in vitro antiproliferative activities against human melanoma cell line A375 were tested and the effect of substituents on the pyrimidinyl ring side chain was investigated.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Discovery of substituted 4-pyrazol-2-benzoxazole-pyridine derivatives as novel c-Met kinase inhibitor

이강진, *이종국, **한선영, *정희정, ***류재욱, *하재두, ****이정옥, *김형래, *조성윤

*충남대 화학과 *한국화학연구원 난치성질환치료제연구센터 **한국화학연구원 약리활성연구센터 ***한국화학연구원 바이오소재연구센터 ****한국화학연구원 항암제연구센터*

Receptor tyrosine kinase (RTK) family is an attractive target for cancer therapy. C-Met kinase is a member of this family with its ligand, hepatocyte growth factor (HGF) or scatter factor (SF) which is crucial for normal mammalian development. c-Met is known to be over-expressed and mutated in a variety of human cancer types. c-Met is accountable proliferation, scattering, invasion, and metastasis of tumor cells. In an effort to search of c-met kinase inhibitors, substituted pyrazolo-benzoxazole derivatives were synthesized and evaluated toward c-met kinase inhibitory activity. Some of the compounds showed moderate activity in vitro enzymatic and cell-based assay.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Identification of MPTP Blocker for the Treatment of Alzheimer's Disease

Mohammad Neaz Morshed

KIST

The MPT refers to the massive swelling and depolarization of mitochondria that occurs under some conditions, most notably as a result of calcium overload and oxidative stress. The cause of the MPT is the opening of a non-specific pore in the inner mitochondrial membrane, known as the mitochondrial permeability transition pore (MPTP). The exact molecular composition of the MPTP is still under debate. The adenine nucleotide translocator (ANT) in the IM, cyclophilin D (Cyp-D) in the matrix, and perhaps the voltage-dependent anion channel (VDAC) in the OM are structural components but other proteins such as benzodiazepine receptor can play regulatory roles. MPTP is drawing tremendous interest now because of its suggested role in cell death which has relevance with Alzheimer's disease (AD). It is suggested that developing drugs targeting neuronal Cyp-D may be a very promising therapeutic strategy to combat Alzheimer's disease. Unfortunately, there are currently no safe Cyp-D inhibitors specific to the brain that could be used to treat Alzheimer's disease in humans. These findings and enigma about the mechanism of MPTP led us to identify novel inhibitors by ligand-based virtual screening using PBR agonists. The role of agonists in the inhibition of MPT is experimentally proved. In the present work, we developed ligand-based pharmacophore to identify novel inhibitors from commercial databases (namely, ChemDiv and Asinex) consisting of 1 047 671 compounds. The selected 110 hits are under processing of biological test.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
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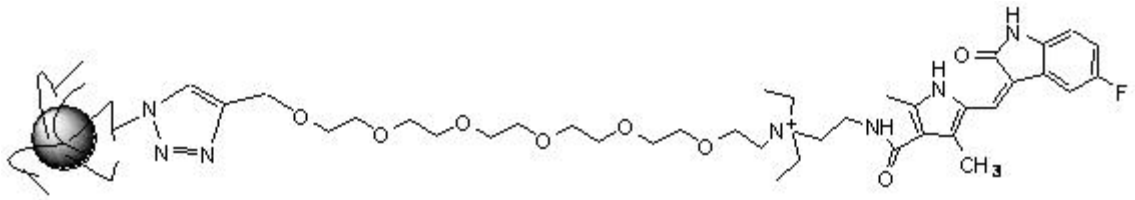
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of Targeted MRI contrast agents via conjugation of MION(Monocrystalline iron oxide nanoparticles) and sunitinib as tyrosine kinase inhibitor

노광태, *김정곤, **이창경

*세종대 화학과 *울산대 영상의학과 **울산대 의과학과*

Magnetic nanoparticles(MNPs) represent a class of non-invasive imaging agents that have been developed for magnetic resonance(MR) imaging. These MNPs have traditionally been used for disease imaging via passive targeting, but recent advances have opened the door to celluar-specific targeting, drug delivery, and multi-modal imaging by these nanoparticles. Targeted nanoparticles were synthesized via conjugation of the functionalized surface of the dextran coated MION(Monocrystalline iron oxide nanoparticles) and sunitinib as tyrosine kinase inhibitor. Functionalized–PEG(polyethylene glycol) was used as the cross-linking agents that have non-toxic, non-immunogenic, hydrophilic and highly flexible properties. In two cell lines, T2 values of sunitinib-CLIO conjugate, sunitinib and saline were measured, and the contrasting effect of the targeted reagent will be described.



일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **MEDI.P-48**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Enhanced Iontophoretic Delivery of Magnesium Ascorbyl Phosphate in Hairless Mice Skin

김수희, *한인숙

*경북대 의과대학 면역학연구실 *경북대 면역학교실*

MAP is known as whitening reagent and hair growth promoter. Since MAP is a highly hydrophilic ionic molecule, it is not easy MAP to deliver into skin. Thus, iontophoretic method was introduced to enhance the MAP penetration by electric repulsion effects. In this study, it was found that iontophoretic delivery of MAP was highly efficient depending on the conditions such as electric currents, application time, drug concentration, and kinds of solution. HPLC is used to analyze the MAPs in samples from the experiment using franz diffusion cell mounted with hairless mice skin. Reverse phase C18 column and the moving phase of aqueous buffer:MeOH = 85:15 were used.

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Synthesis of MPEP derivatives as mGluR modulator

이지연, *강순방, 정낙철, *김유승, **금교창

*고려대 화학과 *KIST 생화학물질연구센터 **KIST 케모인포메틱스연구센터*

Glutamate is the predominant excitatory neurotransmitter in the brain and activates two major receptor classes: the ionotropic glutamate(iGluR) and the metabotropic glutamate receptors (mGluR). mGluRs typically play a regulatory role on fast glutamatergic effects by modulating the ion channel activity and/or neurotransmitter release. And there are eight subtypes of mGluR (mGluR 1-8). Among them, mGluR5's over stimulation has been implicated in numerous CNS disorders.2-methyl-6-(phenylethynyl)pyridine (MPEP) is well known potent and selective noncompetitive mGluR5 antagonist. So we, in an attempt to develop novel mGluR5 antagonists as potential therapeutic agents for neuropathic pain, prepared a series of MPEP derivatives.

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Novel Dihydropyridinyl acetamide and Piperidinyl acetamide derivatives; their synthesis and biological activities as T-type calcium channel blocker

이주현, *강순방, *김유승, 정낙철, **금교창

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T-type Ca2+channel play important role in modulating neuronal excitability on the central and peripheral neuron system, and is the essential intermediary of hormon secrection. However, hyperactivity of T-type calcium channel generate neurological disorders such as epilepsy, hypertension and neuropathic pain. So, T-type Ca2+channel blockers has been researched on a great number of fields. Therefore, we tried to study on the new drug, which is active on T-type Ca2+ channel with good selectivity as a neuropa-thic pain therapy. A series of novel dihydropyridinyl acetamide and piperidinyl acetamide derivatives were designed and synthesized based on the 3D pharmacophore model constructed with known T-type Ca2+channel blockers. The compounds were studied for the evaluation of in-vitro inhibitory activities with α1G and α1H channel in FDSS assay system. Some selected compounds were further studies the selectivity against hERG channel. Hence, we'll discuss the structure-activity relationship.

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Simultaneous determination of dibasic amino acids following trimethylsilyl-trifluoroacyl derivatization on human plasma using GC-MS-SIM

정현수, *윤혜란

*덕성여대 생의약분석실 *덕성여대 생의약분석*

Abstract A rapid analytical method was developed to quantify dibasic amino acids (ornithine, lysine, and arginine) after two-step derivatization procedure with good sensitivity and specificity on human plasma. If early diagnosis is not made, patients with metabolic disorders as HHH syndrome, Hyperornithinemia, and dibasic aminoaciduria rapidly progress to sudden death, physical defect or mental retardation resulted in storage of the toxic material into the brain. Therefore, it is necessary to develop the analytical method for rapid screening and/or correct confirmation diagnosis. The formation of trimethylsilyl derivative (TMS) of the carboxylic (COO-) functional group was performed by adding MSTFA. And then 5 μL of methyl orange was added to the residue until the color was changed to yellow. Consecutively, the trifluoroacyl (TFA) derivative of the amino (-NH2) functional group was produced by adding MBTFA. GC-MS was set with specific ions (m/z 166, m/z 396) of the TMS-TFA derivative of ornithine for selected ion monitoring, lysine (m/z 180, m/z 410), and arginine (m/z 292, m/z 534). A calibration curve showed a linear relationship for the 3 dibasic amino acids in pooled plasma showing 0.9970 ~ 0.9990 in the range of 10 - 400 ng investigated.The utility of the method was demonstrated by quantifying various concentration of fortified dibasic amino acids on normal plasma. The new method was simple with just two step derivatization, time and labor saving without SPE or liquid-liquid extraction. The described method could be useful for routine analysis, monitoring, and clinical diagnostic application of metabolic disorders on dietary therapy with excellent sensitivity and rapidity.

Simultaneous determination of dibasic amino acids following trimethylsilyl-trifluoroacyl derivatization on human plasma using GC-MS-SIM

GC-MS-SIM을 이용한 TMS-TFA 유도체화 후 혈장 중 염기성 아미노산의 동시정량법 개발

Hyunsu Jeong, and *Hye-Ran Yoon

Department of Biomedical & Pharmaceutical Analyses, College of Pharmacy, Duksung Women's University, Seoul, Korea

Abstract

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Key words: GC-MS-SIM, Dibasic amino acids, Trimethylsilylation, Trifluoroacylation, Derivatization, Inherited metabolic disorder

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Synthesis and Evaluation of BMK-Y101, a Potent CDK7 and CDK9 Inhibitor, for Treatment of Human Hepatocellualar Carcinoma

김영종, 권순호, 김병문

서울대 화학부

Serine/threonine protein kinases play important roles in the signal transduction pathways that control the proliferation and differentiation of eukaryotic cells. Cyclin-dependent kinases (CDK's), which belong to the Ser/Thr kinase family, are regulators of eukaryotic cell cycle progression. These kinases phosphorylate various target proteins whose activities are crucial for the cell cycle progression. The cell cycle is controlled by the mechanisms that operate at checkpoints in the G1 and G2 phases. These mechanisms involve complex interactions among many proteins, including CDK's.BMK-Y101 is a new pyrrolopyrimidine-based inhibitor, which exhibits strong inhibition activity of CDK7 and CDK9. Inhibition of CDK7 and CDK9 exerts consequent negative effects on RNA synthesis, which strongly promotes apoptosis. In vivo evaluation in mice corroborated the anticancer potential of BMK-Y101 against human hepatocellular carcinoma (HCC) model.

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Synthesis of New Purpurinimide-Hydrazone Conjugates

Li Jia Zhu, *Cui Bing Cun, **박호성, **심영기

*인제대 나노시스템공학과 *인제대 나노공학과 **인제대 나노공학부*

The synthesis of the new Chlorin-EGCG Conjugates which can be used as photosensitizers in PDT is done by modification of 17-methyl ester group of chlorophyll-a derivatives such as methyl pyropheophorbide-a (Mppa), purpurin-18 and purpurinimide. The structures of new chlorophyll derivatives were characterized by UV, IR, 1H NMR spectra and elemental analysis. Their in vitro anticancer activities were also tested on A549 lung cancer cell model. Keywords: chlorin-EGCG conjugates, chlorophyll-a derivative, photodynamic therapy (PDT)

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Synthesis and in vitro Anticancer Activity Study of the New Chlorin-EGCG Conjugates

Li Jia Zhu, *Cui Bing Cun, **박호성, **심영기

*인제대 나노시스템공학과 *인제대 나노공학과 **인제대 나노공학부*

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SYNTHESIS AND ANTIBACTERIAL ACTIVITY EVALUATION OF INDOLEAMINE COMPOUNDS ANALAGOUS TO API -1252 AS FAB INHIBITORS

Deepak Bhattarai, *배애님, **금교창

*과학기술연합대학원대 organic chemistry *KIST 생체과학연구본부 **KIST 케모인포메틱스연구센터*

The increasing use of antimicrobials has resulted in many pathogens developing resistance to the existing powerful drugs. Consequently, there is a pressing need to develop new antibiotics to keep place with bacterial resistance. Recent advances in microbial genomics and X-ray crystallography provide opportunities to identify novel antibiotic targets for the development of new classes of antibiotics and to design more potent antimicrobial compounds derived from existing antibiotics respectively.The indoleamine compound show broad-spectrum antibacterial activity by targeting the fatty acid biosynthetic pathway through inhibition of enoyl-acyl carrier protein reductase and provides a potential scaffold for the development of new broad spectrum antibiotics. We use the similar scaffold and synthesize the analogous compounds according to the recommendation of molecular modeling team.

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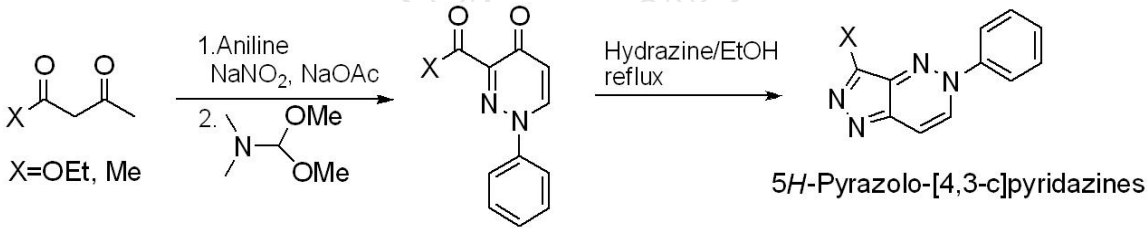
5H-Pyrazolo[4,3-c]pyridazine: Synthesis of a novel heterocycle

양은혜, *윤우섭, **김정근, ***최지원, 이종국, ****한선영, 조성윤, *****이정옥, 김형래, 하재두

*한국화학연구원 난치성질환치료제연구센터 *레고캠바이오 화학과 **고려대 화학과 ***서강대 화학과 ****한국화학연구원 약리활성연구센터 *****한국화학연구원 항암제연구센터*

The synthesis of novel heterocycles is of going interest to the medicinal chemistry and pharmaceutical communities because heterocycles are common in drugs and possess biological activity against various drug targets. In our laboratories we recently had need to prepare 5H-pyrazol[4,3-c]pyridazine heterocyclic system for the development of kinase inhibitors. Herein, we describe an efficient synthesis of the novel 5H-pyrazol[4,3-c]pyridazines from 2,4-dione systems.



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Metabolic profiling of catecholamines and their metabolites in biological fluids by gas chromatography-mass spectrometry

홍주연, *홍종기

*경희대 약학대학 *경희대 약학과*

The measurement of catecholamines and their metabolites in biological samples is very useful for clinical diagnosis of several diseases such as Parkinsons's disease, pheochromocytoma, or neuroblastoma. Gas chromatography/mass spectrometry (GC/MS) was employed for quantitative analysis using isotopically labeled-internal standards. Solid-phase extraction with MCX-cartridges as cleanup method was applied for the extraction of acidic and basic catecholamines in biological fluids. After cleanup, two-step derivatization with MSTFA and MBHFBA was used for silylation and acylation of catecholamines. Calibration curves showed good linearity between 1.0 and 1000.0 ng/mL, with a correlation coefficient ≥ 0.99. The limits of quantification of catecholamines were in the range of 0.07 ~ 0.38 ng/mL. The mean recovery rate of each compound ranged from 88 to 110%. The principal component analysis (PCA) combined with GC/MS chromatographic data was performed for observation of metabolic perturbations of catecholamines and their metabolites in biological fluids. Based on PCA, several potential biomarkers (catecholamines and their metabolites) will be found to clinically diagnose a specific disease.

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Synthesis and biological evaluations of 4-[2-(4-bromo-phenylsulfanyl)-acetylamino]-1-phenethlyl-1H-pyrazole-3- carboxylic acid as a novel class of FAF-1(Fas Associated factor) induced cell death inhibitors

이서현, 서지희, 이규양

한국화학연구원 대사증후군치료제연구센터

Ischemia, a symptom of reduced blood supply to organs or tissues, is caused by contraction or occlusion of the blood vessels. Fas-mediated cell death has been shown to be induced after ischemic injury. As part of our medicinal chemistry research program, we identified new inhibitors of ischemic cell death by high-throughput screening of the ischemia-induced Fas-mediated pathway. It was found that 4-[2-(4-bromo-phenylsulfanyl)-acetylamino]-1-phenethyl-1H-pyrazole-3-carboxylic acid is noble structure as ischemic cell death inhibitors. Synthesized compounds were biologically evaluated using in vitro H9c2 cell and in vivo MCAO models. Pharmacological activities correlated with their structures will be presented.

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Evaluations of 5-[^{18}F]Fluoropentyltriphenylphosphonium Salt as Novel Mitochondrial Voltage Sensor in Rat Myocardial Infarction Model

김동연, 김희정, 도보영, 유국현

동국대 화학과

Despite substantial advances in the diagnosis and treatment of cardiovascular diseases, there are a few radiopharmaceuticals for diagnosis of ischemic heart diseases (IHD) using PET. Thus, we synthesized 5-[^{18}F]fluoropentyltriphenylphosphonium salt (5-[^{18}F]FPTP), that specifically accumulates in myocardial cells according to mitochondrial membrane potential. Here, we evaluated the performance of 5-[^{18}F]FPTP as a mitochondrial voltage sensor *in vitro* and *in vivo*. We evaluated cell uptake of 5-[^{18}F]FPTP in embryonic cardiomyoblast cell line (H9c2). The uptake of 5-[^{18}F]FPTP, [^{3}H]tetraphenylphosphonium ([^{3}H]TPP) and [^{99m}Tc]sestamibi was examined after modulation of mitochondrial membrane potential with CCCP (carbonyl cyanide m-chlorophenylhydrazone). 5-[^{18}F]FPTP and [^{3}H]TPP were more sensitive in the change of mitochondrial membrane potential than [^{99m}Tc]sestamibi. We assessed biodistribition of 5-[^{18}F]FPTP in normal BALB/c mice (n = 12) that showed high accumulation in the heart (12.02 ± 3.63 ID%/g , at 10 min). Dynamic micro PET study showed high accumulation and retention in the heart and very rapid clearance from the liver. Heart-to-liver ratio was over 1.0, 2.0, and 3.0 after 2 min, 10 min, and 20 min of tracer injection, respectively. Micro PET study in myocardial infarction rats showed decreased uptake of 5-[^{18}F]FPTP in the region of hypoperfusion confirmed by 2,3,5-Triphenyltetrazolium chloride (TTC) staining. Quantitative analysis revealed high correlation between micro PET image and TTC staining (r^2=0.85).5-[^{18}F]FPTP was sensitive in mitochondria membrane potential and allows quantitative assessment of regional myocardial ischemia or infarction. 5-[^{18}F]FPTP might be useful for clinical cardiac PET/CT applications.

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Bromopyrrole alkaloids from a tropical marine sponge *agelas* sp

김창권, *이연주, 원호식, **이희승

*한양대 응용화학과 *한국해양연구원 해양바이오센터 **한국해양연구원 해양천연물연구실*

Bromopyrrole alkaloids are known to have a variety of biological activities such as antimicrobial activity, tyrosine kinase inhibitory activity and antifouling activity. During our research for the discovery of bioactive substances from marine sponges collected from Chuuk, Federated State of Micronesia, we have examined *agelas* sp. which are known to be an abundant source of various bromopyrrole alkaloids. We have isolated dibromophakelline, spongiacidin, septrin and one unidentified compound expected to have bromopyrrole in its structure. The structures of isolated compounds were elucidated by means of spectral methods including 2D NMR and MS.

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Isolation of cytotoxic sesterterpenoid suvanine from a tropical marine sponge

이정우, *이희승, **이연주

*인하대 화학과 *한국해양연구원 해양천연물연구실 **한국해양연구원 해양바이오센터*

In the course our research for the discovery of bioactive substances from marine sponges collected from Chuuk, Federated States of Micronesia, we have encountered a sponge of which the extract exhibited significant cytotoxity against human leukemia cell line. A careful investigation of chemical composition revealed that the extract contains large amount of suvanine, a sesterterpene sulfate reported to have inhibitory activity against thrombin and trypsin. The IC_{50} value of suvanine was 31.6 μg/mL, which suggests that the cytotoxicity of the extract results from suvanine. Other sesterterpenoids expected to have structures analogous to suvanine were also obtained and their structures are under investigation.

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Synthesis of 3-alkylamino-1,2-naphthoquinones as the key intermediate for the construction of perylenequinone core

김범태, *송춘호, **한인철, **방성준, *조익수, *황기준

*전북대 생리활성물질연구소, 생리활성소재과학과 *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. As our continuing program to develop new perylenequinone class of compounds with diverse substitution pattern at 1, 12-position and their variation in photosensitizing activity, we synthesized 3-alkylaminonaphthalene derivatives and in sequence converted them to the corresponding 3-alkylamino-1,2-naphthoquinones, the key intermediate for the construction of perylenequinone core.

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5-Hydroxyindole alkaloids isolated from the tropical sponge *Hyrtios* sp. and the East Sea marine sponge *Psammocinia* sp

이동근, *김창권, **이연주, ***이희승

*한국해양연구원 해양바이오연구센터 해양천연물연구실 *한양대 응용화학과 **한국해양연구원 해양바이오센터 ***한국해양연구원 해양천연물연구실*

In the course of our study on the chemical investigation of marine organisms, we found indole alkaloids from the sponge *Hyrtios* sp. collected in Chuuk State, Federated States of Micronesia and the sponge *Psammocinia* sp. collected at Dokdo Island, Korea. From the extracts of *Hyrtios* sp., 1-carboxy-6-hydroxy-3,4-dihydro-β-carboline, 6-hydroxy-3,4-dihydro-1-oxo-β-carboline, 5-hydroxy-1H-indole-3-carboxylic acid methyl ester, serotonin, hyrtiosin A, 5-hydroxyindole-3-carbaldehyde, and hyrtiosin B were isolated. And bis-indole alkaloid, hyrtinadine A together with other known metabolites were isolated from the extracts of *Psammocinia* sp.. A structure of the new compound was elucidated by spectroscopy method including mass spectroscopy and 2D NMR spectroscopy.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표종류: 포스터, 발표일시: 금 10:30~12:30

New Macrocyclic DTPA-bis(amide) Functionalized by tranexamic methyl ester: Synthesis, Complexation and stability properites

구성욱, *양은지, *김태정

*경북대 응용화학과 *경북대 응용화학과*

New macrocyclic DTPA-bis(amides) functionalized by tranexamic methyl ester and theirGd(III)-complexes were prepared and characterized by analytical and spectroscopic techniques. Potentiality of complex as contrast agents for magnetic resonance imaging (MRI CA)was investigated by measuring relevant physicochemical properties and relaxivities and compared with[Gd(DTPA-BMA)(H2O)] (DTPA-BMA=N,N''-di(methylcarbamoylmethyl)diethylenetriamine-N,N',N''-triacetate)(Omniscan). The R1 relaxivity of aqueous solutions of complex is 10.5 s-1mM-1 which is comparable with those of Omniscan (r1=4.58 mM−1sec−1).

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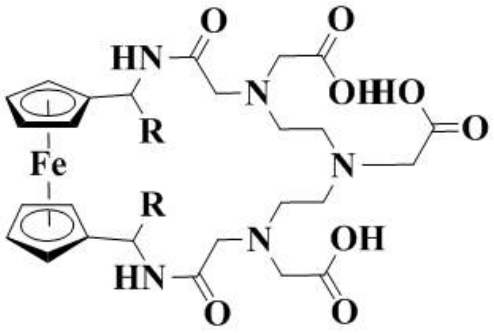
Gd-DTPA Conjugates of 1,1'-bis(amino)ferrocenes as Novel MRI Blood-Pool Contrast Agents

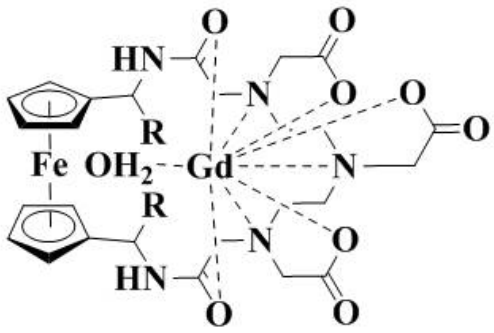
김희경, *정기혜, **Patel Mehulkumar, 강민경, *김태정

*경북대 의용생체공학과 *경북대 응용화학과 **경북대 화학과*

Contrast-enhanced magnetic resonance angiography (CE-MRA) is well established for the diagnosis and management of vascular disease. Standard extracellular contrast media are currently used for almost all CE-MRA applications. During steady state, however, angiography is not useful because of rapid extravasation of such extracellular contrast media resulting in decreasing vascular and increasing background signal. Recently, a new generation of contrast agents with intravascular distribution, also refered to as blood pool contrast agents (BPCAs), has become available. The BPCAs provide strong and prolonged vascular enhancement. Herein, We report the synthesis of macrocyclic DTPA conjugates of 1,1'-bis(amino)ferrocenes (1a-b) and their Gd-complexes [Gd(L)(H_2O)] (2a-b, L = 1a-b) for use as new MRI blood-pool contrast agents. High R_1 relaxivity in HSA as well as high thermodynamic and kinetic stabilities is obserevd with 2a.



1a-b



2a-b

a: R=Me
b: R=Ph

대한화학회
THE KOREAN CHEMICAL SOCIETY

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장소: 대구엑스코
발표코드: **MAT.P-1**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

The attachment of CdS quantum dot to graphene oxide by covalent bonding

TUAN ANH PHAM, 정연태

부경대 이미지시스템공학과

The fabrication of carbon-based materials with semiconductor quantum dot is one of the most important topic of nanotechnology due to such materials have potential optoelectronic applications. In this study, hybrid nanomaterial of covalently immobilized graphene oxide (GO) with CdS quantum dot was prepared by a facile approach for the first time. Pristine graphite was firstly oxidized in order to obtain carboxylic acid functionalized GO, which was further acylated with thionyl chloride to give acyl chloride bound GO surface. Then, the CdS quantum dot was modified using 4-aminothiolphenol to introduce amino groups on its surface. Subsequently, the attachment of CdS quantum dot onto the GO surface was obtained via amidation reaction between amino groups of surface-functionalized CdS and acyl chloride groups of GO.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Energy Transfer at Graphene-MoS_2 Single-Layer Composites

권혁상, *류순민, **김성근

*서울대 화학부 *경희대 응용화학과 **서울대 화학부 & 생물물리 및 화학생물학과*

Photoluminescence (PL) of molecules near metallic surfaces is strongly quenched via either fluorescence resonance energy transfer or charge transfer. In this study, we investigated PL of a single MoS_2 layer in direct contact with graphene, a two-dimensional metal. An atomically thin MoS_2 film with a strong PL due to a direct band gap unlike in its bulk form holds a great potential in optoelectronic applications. Graphene-MoS_2 single-layer composites were prepared by mechanical exfoliation of MoS_2 followed by deposition of a single-layer graphene. We examined the dependence of PL efficiency of single- and few-layer MoS_2 films on graphene over-layer. This study on energy transfer between truly two-dimensional semiconductor and metal composite systems have great implications for future optoelectronic and photovoltaic applications.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Optical properties of pyrene-labeled gold nanoparticles

이현진, 이동일

연세대 화학과

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 facilitate functionalization, we have synthesized amine-terminated MPCs with different thiolates; L-glutathione, L-cysteine, by a modified Brust's synthesis. The amine-terminated MPCs were amide coupled with pyrene-NHS (pyrrolidin-1-yl pyrene-4-carboxylate) to prepare chromophore-functionalized MPCs. Pyrene loading on gold MPCs was varied by controlling the reaction condition and quantified by UV/Vis absorption spectroscopy. Pyrene-labeled gold MPCs were characterized using transmission electron microscopy (TEM), UV-vis absorption and fluorescence spectroscopy. The fluorescence of pyrene is often quenched in the proximity of gold surface as a result of excited-state interactions. The fluorescence quenching of the pyrene-labeled MPCs is compared as a function of the pyrene-gold linker and pyrene loading.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Metal oxide photocatalysts modified with monolayer-protected metal clusters

이명순, 이재일, 이동일

연세대 화학과

Noble metal deposits on the surface of semiconductor metal oxides such as TiO_2 and ZnO are known to increase the photocatalytic efficiency of the metal oxides by increasing electron/hole separation. A few reports have explored the use of monolayer-protected gold clusters (MPCs) as well-defined metal deposits on semiconductor photocatalysts. However, the role of metal deposits on surface of semiconductor and the effects of the ligands in the use MPCs in photocatalysis is yet to be fully understood. In this presentation, TiO_2 nanoparticle photocatalysts modified with uniform gold nanoparticles are prepared by anchoring bifunctional glutathione-coated MPCs onto TiO_2. The photocatalytic degradation of Uniblue A (UBA) is carried out with thus prepared MPC-TiO_2 composites, which show, however, no enhancement upon anchoring of MPCs. The MPC-TiO_2 composites are thermally treated to activate the catalytic activity. When the MPC-TiO_2 composites are calcined at 250 °C, the glutathione ligand on gold surface is partially removed and the photocatalytic activity of the composites significantly increases, highlighting the role of gold in the photocatalytic reactions. However, when the calcination temperature is raised to 400 °C, the photocatalytic activity of the composites drastically decreased. X-ray photoelectron spectroscopy analysis of the calcined composites reveals that significant amount of oxidized sulfur remains after calcination that appears to act as a recombination center for the photogenerated electrons and holes, resulting in drastic decrease in the photocatalytic activity. These results emphasize the important role of ligands in the use of MPCs in photocatalysis.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Superhydrophilic and hydrophobic modification of antireflective $La(OH)_3$ nanorod films

유지호, 변송호

경희대 화학과

$La(OH)_3$ nanorods were self-stacked on the glass slide substrates using an aqueous suspension obtained from the hydrolysis of LaOCl. These thin-film coatings of $La(OH)_3$ nanorods led to a significantly reduced reflective losses in the visible region, exhibiting an attractive and potentially useful single-layer antireflection property. Furthermore, $La(OH)_3$ nanorod layer provides a sufficiently porous and rough surface required to achieve superhydrophilicity and hydrophobicity. When SiO_2 nanoparticles of ca. 20 nm in diameter were deposited onto $La(OH)_3$ layer of high roughness, the resulting $La(OH)_3/SiO_2$ film demonstrated an interesting nanoporosity-derived superhydrophilicity and antifogging property with no significant loss of antireflective property. Interestingly, preliminary results indicated that the porous $La(OH)_3$ film coated with poly(dimethylsiloxane) (PDMS) exhibits highly hydrophobic and antireflective property.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of Pd nanoparticles well dispersed on the layered yttrium hydroxide nanosheets

이은수, 변송호

경희대 화학과

As a supporting materials for Pd nanoparticles, well crystallized layered yttrium hydroxide (LYH), $Y_2(OH)_5Cl{\bullet}nH_2O$, has been synthesized by the hydrothermal reaction. LYH^-supported nanopalladium(0) catalysts are prepared by an exchange reaction between interlayer Cl^- and $PdCl_4^{2-}$ followed by reduction. When $PdCl_4^{2-}$/LYH was reduced with hydrazine hydrate in distilled water, the formation of Pd nanoparticls (2-5 nm in average diameter) was induced on the surface and at the edge of LYH sheets. In contrast, when reduced with H_2 gas at 150 °C, an accompanying exfoliation led to well dispersed Pd nanoparticles on the exfoliated monolayers of LYH. The catalytic activity of Pd/LYH is compared with those of commercial Pd/C, Pd/SiO_2, Pd/Al_2O_3catalysts.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Self-assembly of grafted hydroxocation nanosheets to the layered gadolinium hydroxide

이병일, 변송호

경희대 화학과

The layered rare-earth hydroxides (LRHs) are not only able to be delaminated into nanosheets, but also to be reconstructed to their layered stuructures with suitable counter anions. In this study, the layered gadolinium hydroxide (LGdH) was synthesized by co-precipitation method and then exfoliated to the hydroxocation nanosheets in aqueous solution. To restack the nanosheets, the dodecyl sulfate was selected as an anionic glue and self-assembly of the hydroxocation nanosheets was attempted at ambient temperature. In the pH dependent assembly process, the grafting of dodecyl sulfate anions on the gadolinium hydroxide nanosheets was observed at pH < 7. As the concentration of H^+ ions is gradually increased in solution, the protonated OH groups on the gadolinium hydroxide sheets seem to be replaced by sulfate anions. In contrast to when exchanged into the interlayer space of LGdH by host-guest reaction, the sulfate groups grafted on the gadolinium hydroxide layers formed $Gd_2(SO_4)_3$ phase at 250℃ and then transformed to $Gd_2O_2SO_4$ structure at higher than 600 ℃.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of Gold Nanoparticles: A Novel Approach by Using a Macrocycle

Thathan Premkumar, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과 나노바이오전자재료공학과*

A significant feature of nanoscience and nanotechnology concerns the progress of experimental protocols for the preparation of nanoparticles of diverse chemical compositions, sizes, shapes, and controlled dispersity and without environmental risks. Here we report a facile and one-pot synthesis of well dispersed gold nanoparticles by the reaction of an aqueous potassium tetrachloroaurate(III) solution with a macrocycle at room temperature without applying any kind of traditional reducing agents and/or external energy. The gold nanoparticles could be isolated and redispersed in aqueous solution and the synthetic procedure presented here is easy, green, and user-friendly

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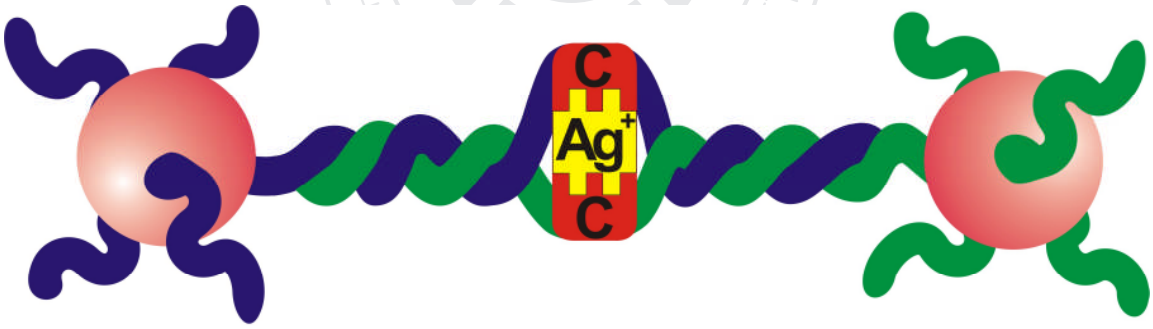
발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

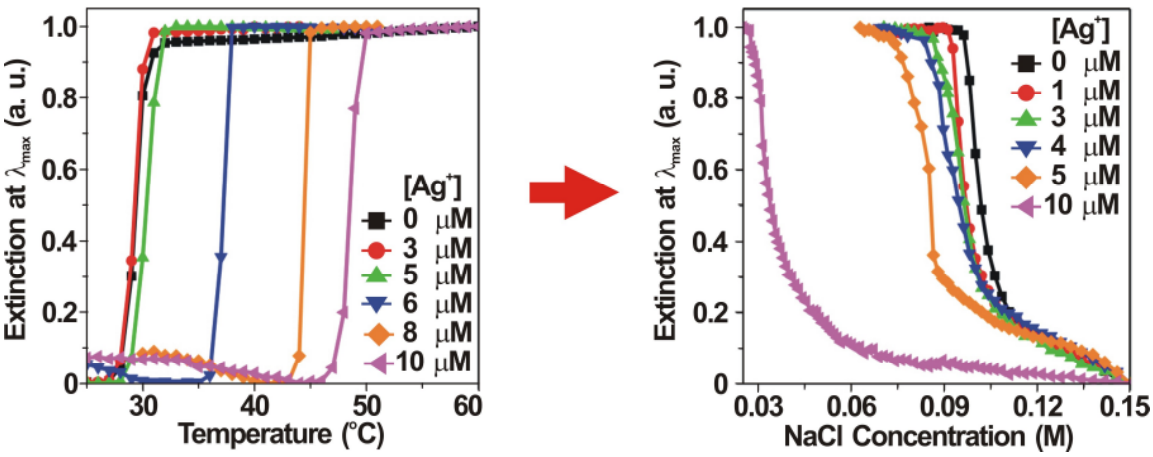
Salt concentration-induced dehybridization of DNA–gold nanoparticle conjugate assemblies for diagnostic applications

오주환, 이재승

고려대 신소재공학부

We present the cooperative dehybridization of DNA–gold nanoparticle conjugate (DNA–AuNP) assemblies induced by reduced salt concentration ([salt]), which can be precisely controlled by various conditions. The detection of Ag^+ based upon the [salt]-induced dehybridization of DNA–AuNP assemblies is five times more sensitive than that achieved under conventional thermal melting conditions.





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발표종류: 포스터, 발표일시: 목 10:30~12:30

Controlling the Stacking of TTF Molecules in a Microcrystalline Porous Coordination Network

NAZRUL ISLAM, *Javier Martí-Rujas, *Makoto Fujita, Masaki Kawano

Division of Advanced Materials Science Pohang University of Science and Technology (POSTECH)
**Department of Applied Chemistry School of Engineering The University of Tokyo*

Despite the wide variety of applications found in porous coordination networks conductivity still remains unexplored. Tetrathiafulvalene (TTF) and related molecules have attracted much attention as electronic devices due to their widespread potential and versatility through incorporation of the π-rich redox-active building block into materials. One important aspect to emerge conductivity is the controlling of arrangement (packing) of TTF molecules, as it is crucial to bring the S···S distances between the molecules close enough to allow charge mobility. We have synthesized porous coordination network which successfully encapsulates TTF molecules as a guest. The details structure and the stacking of TTF molecules in the confined space of porous coordination networks will be discussed.

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발표분야: 재료화학
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Adsorptive Removal of Methyl Orange from Contaminated Water with Metal-organic Frameworks

강인중, **Enamul Haque,** 정성화

경북대 화학과

Metal-organic frameworks (MOFs) attract considerable attention because of huge porosity, and easy tunability of their pore size/shape and many potential applications [1]. Two typical highly porous MOF materials based on chromium benzenedicarboxylates (Cr-BDC) with special structure of MIL-101 and MIL-53 have been used for the adsorptive removal of methyl orange (MO), a harmful anionic dye, from aqueous solutions. The adsorption capacity and adsorption kinetic constant of MIL-101 are greater than those of MIL-53, illustrating the importance of porosity and pore size for the adsorption. The performance of MIL-101 improves with modification: the adsorption capacity and kinetic constant are in the order of MIL-101 < ethylenediamine-grafted MIL-101 < protonated ethylenediamine-grafted MIL-101 (PED-MIL-101) even though the porosity and pore size are slightly decreased with grafting and further protonation. The adsorption capacity of PED-MIL-101 decreases with increasing the pH of an aqueous MO solution. These results suggest that the adsorption of MO on the MOF is at least partly due to the electrostatic interaction between anionic MO and a cationic adsorbent. Adsorption of MO at various temperatures shows that the adsorption is a spontaneous and endothermic process and that the entropy increases with MO adsorption. The adsorbent MIL-101s are re-usable after sonification in water. Based on this study, MOFs can be suggested as potential re-usable adsorbents to remove anionic dyes because of huge adsorption capacity, facile modification and ready re-activation [2].

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile syntheses of SAPO-34 molecular sieves with microwave heating: effect of reaction conditions

전종원, 정성화

경북대 화학과

Various reaction conditions including temperature, time and type and concentration of templates have been changed in order to facilely synthesize, especially with microwave (MW) heating, SAPO-34 molecular sieves. SAPO-34 molecular sieves can be synthesized rapidly with MW irradiation from a gel containing tetraethylammonium hydroxide (TEAOH) as a template. However, other several templating molecules lead to SAPO-5 molecular sieves under MW irradiation even though SAPO-34 is obtained by conventional electric synthesis from the same reactant gels. Moreover, SAPO-34 can be obtained more easily by increasing the TEAOH or silica concentration or by increasing the reaction temperature. SAPO-34 can be obtained within 5 min in a selected condition (high temperature of 210 oC) with MW heating, which may lead to a continuous production of the important material. SAPO-34 synthesized by MW irradiation is homogeneous and small in size and beneficial in an acidic catalysis like dehydration of n-butanol.

일시: 2010년 10월 14~15일(목~금) 2일간
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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Microwave-synthesis of porous chromium-benzenedicarboxylates: phase-conversion and phase-selectivity

Nazmul Abedin Khan, 전종원, 정성화

경북대 화학과

Two porous chromium-benzenedicarboxylates, denoted as MIL-53 and MIL-101, has been synthesized with both conventional electric (CE) and microwave (MW) heating to understand phase-selectivity and phase-transition between these solids. One chromium benzenedicarboxylate, the kinetically favorable MIL-101 is the phase obtained at the early stage of the reaction while thermodynamically favorable MIL-53 phase is obtained at the expense of MIL-101 at longer synthesis time. Phase-transition from MIL-101 to MIL-53 occurs by an indirect conversion. At the longer synthesis time the MIL-101 is degraded, and subsequently, MIL-53 is observed via the reorganization of the decomposed species. Moreover, it is suggested that MW irradiation provides a phase-selective synthesis of MIL-101 due to rapid synthesis, preventing the conversion into the thermodynamically favorable phase (MIL-53). Therefore, the MW synthesis may lead to a new/facile way to find new metal-organic frameworks (MOFs) especially that is hard to synthesize due to a conversion into a more stable phase or dense phase without porosity.

일시: 2010년 10월 14~15일(목~금) 2일간

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Ultrasound-aided syntheses of porous isostructural lanthanide-benzenetricarboxylates (Ln-BTC) at room temperature

Nazmul Abedin Khan, 강인중, 전종원

경북대 화학과

Several porous isostructural [Ln(BTC)(H2O)•4.3H2O] or Ln-BTCs (Ln: Ce, Tb and Y; BTC stands for 1,3,5-benzenetricarboxylate) have been synthesized by ultrasonic irradiation at ambient condition. The syntheses under ultrasound accelerated much to get the fully crystallized phase in minutes only. Moreover, the particle size can considerably be decreased by this method. Based on the XRD, FE-SEM and surface area, it can be understood that the Ln-BTCs are homogeneous in phase, isostructural and microporous. The synthesis rates are rCe-BTC > rTb-BTC > rY-BTC for both in the nucleation and crystal growth stages, illustrating the importance of lability of the metal ions in the synthesis of the MOF materials. It is believed that these lanthanide MOFs having high porosity and/or luminescent property should be multifunctional materials.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

A Novel Synthesis of Small Silica Nanoparticles with Fluorescence Dye for Biomedical Application

장혜윤, 박원철

서울대 융합과학기술대학원 나노융합학과

Silica nanoparticles have attracted tremendous attention in biomedical research area due to their low toxicity, easy modification, inexpensive process, etc. In this work, we report on the synthesis of fluorescence dye embedded silica nanoparticles by sol-gel process. This approach enables to prepare monodispersed core silica nanoparticles in the range of 20-50 nm. By further coating process, silica nanoparticles with shells of uniform and desired thickness are obtained. In addition, mesoporous layers are further grown around core particles. The as-prepared nanoparticles show advantages of photoluminescence signaling and structural aspects than previous one and are expected to be widely applicable to biomedical imaging and drug delivery.

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Fabrication of uniform mesoporous carbon nanospheres by using the silica nanoparticles as templates

권파, 박원철

서울대 융합과학기술대학원 나노융합학과

A novel process was developed for the synthesis of uniform mesoporous carbon nanospheres with large surface area and well dispersibility. The monodispersed silica nanoparticles were used as starting materials and octadecyltrimethoxysilane as porogen agent to create core-shell nanostructures. The composite was carbonized under inert gas, and the silica was etched away by using sodium hydroxide solution. The monodispersed morphology of the mesoporous carbon nanospheres was confirmed by transmission electron microscopy and scanning electron microscopy. The as-prepared carbon nanomaterial showed high Brunauer-Emmett-Teller surface area and large pore volume. The drug loading and release properties were also studied.

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Organic-Inorganic Composite Coated Electrogalvanized Steel Sheet for Digital TV

조두환

(주)포스코 기술연구소 표면처리연구그룹

Recently digital TV industry has been drastically moved the illuminating system, from PDP and LCD to LED, to provide the high-definition image. Due to strong competition, the TV makers would like to reduce the production cost by using low-priced materials such as steels instead of aluminum and plastics *etc*. In this presentation, we have developed new low-priced electrogalvanized steel sheet coated with organic-inorganic composite solution to substitute high-priced aluminum and plastic for the rear cover panel in the digital TV. The coating solution was prepared by ball-milling the mixture solution that consists of high-solid polyester resin, melamine hardener, black pigment, and additives. The composite solution was coated on the steel sheets by using roll coater *via* induction curing furnace. Although the coated layer was 10μm by thickness, comparative conventional PCM steels having 25μm, exhibits excellent quality to use the rear cover panel. The new steel product was applied to get quality certification from the customer (Samsung & LG Electronics). Detailed discussion will be present including the preparation of composite solution, roll coating technology, induction curing and quality evaluation of the product.

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Synthesis of porous carbon material from MOF

임승훈, Dybtsev N. Danil

포항공과대 첨단재료과학부

Recently, study of new porous materials with high adsorption capacity is one of the most interesting issue. Porous carbon materials, such as activated carbon, are good candidate for gas storage because of high surface area, high adsorption capacity and exceptional chemical stability. Herein we report new type of carbon materials which are synthesized from metal-organic framework precursors. The porous carbon materials are characterized by powder X-ray diffraction, SEM images and gas sorption isotherm (N_2, H_2, CO_2). The gas adsorption capacity of reported micro porous carbon is comparable to that of other porous materials such as activated carbons and metal-organic frameworks.

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Growth of nanostructured zinc oxide by the reaction of ZnO powder and carbon monoxide

서상원

영남대 응용화학공학과

ZnO nanostructures with various morphologies such as rod, comb, and cone were prepared by calcination of ZnO powder under a flow of mixed gas of carbon monoxide and nitrogen and characterized by XRD, SEM and TEM. The morphologies depended on the reaction temperature and gas flow rate. The morphology of ZnO nanostructures grown on the fluorine-doped tin oxide (FTO) substrate had an effect on the photoresponse in the photoelectrochemical cells.

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Preparation of well-dispersed reduced graphene oxide sheets using a photochemical method

문건희, 최원용

포항공과대 환경공학부

Herein we prepared well-dispersed and highly reduced graphene oxide sheets in the organic solvent by photocatalytic reduction using 'Polyoxometallate (POM)' as a homogeneous photocatalyst working under UV light irradiation. The reduced graphene oxide by photocatalytic reduction of graphene oxide has been previously synthesized as the composite such as TiO2-reduced graphene oxide. The photo-excited electrons of TiO2 under UV light have been considered as a main source of photocatalytic reduction of graphene oxide. However, we observed that graphene oxide was reduced by organic radical species which were produced from the reaction between the photo-generated holes and alcohols, not by the photo-excited electrons of POM. We also synthesized the composite of the reduced graphene oxide-Ag nanoparticles by injecting AgNO3 under UV light after the complete reduction of graphene oxide.

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The effects of conducting molecular wires in solar energy-converting photoelectrochemical cells

서연주, *이성훈

*서울대 화학과 *서울대 화학부*

The regularly ordered valve metal oxide nanotubes can be formed by our well-established electrochemical anodization processes. Among them, the regular arrays of TiO2 nanotubes are promising candidates for solar energy conversion as a photoelectrochemical cell. Its band position is properly located for water splitting. The regular arrays of TiO2 nanotubes have large surface areas. However, the band gap of TiO2 belongs to the UV portion of a solar spectrum. So, we need to expand its absorption to the visible spectral range by attaching CdS or CdSe quantum dots to titanium oxide nanotubes to enhance solar energy conversion efficiency. Quantum dots originally synthesized are coated with insulating trioctylphosphine or oleic acid which behaves as a barrier to the charge transfer from the CdS or CdSe qunatum dots to the titania nanotubes. With replacing those with conjugated molecules called conducting molecular wires, we investigated their effect on the charge transfer from QDs to TiO2 nanotube arrays under a simulated AM1.5 illumination.

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Novel Asymmetric Oligomers Based on Benzo[d,d´]thieno[3,2-b;4,5-b´]dithiophenes and Solution-Processed Organic Field-Effect Transistors

이동희

경상대 고분자공학과

In this study, We report the synthesis and characterization of a series of extended arylacetylenes, 2[(Hexyloxyl)phenyl]ethynyl- Benzo[d,d´]thieno[3,2-b;4,5-b´]dithiophenes and 2[(phentyloxyl)phenyl]ethynyl Benzo[d,d´]thieno[3,2-b;4,5-b´]dithiophenes were synthesized by a novel route, the key point of which is the acid-induced intermolecular cyclization reaction of aromatic methyl sulfoxides, and were confirmed by 1H-NMR and FT-IR studies. The obtained oligomers showed the good solubility in common organic solvents such as hexane, chloroform, and dimethylchloride at room-temperature, which is due to the introduced alkyl chain. The physical and optical properties of the oligomers were studied using differential scanning scalorimetry (DSC), cyclic-voltammetry (CV), UV-visible absorption and PL studies. Solution processed OTFT device based on synthesized oligomers show a high hole mobility of up to 0.09 cm2V-1s-1, Ion/Ioff of 106 and threshold voltage of –14V

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Synthesis of New Perylene Derivative Containg 2-(naphthalen-2-yl)thiophene Functionalized with Alkyl Groups and Solution Processed OTFT characteristics

LU WANXIANG

경상대 고분자공학과

Solution processed organic thin film transistors (OTFTs) have attracted much attention due to their potential use in low-cost, lightweight, and flexible electronic devices. In thisstudy, we designed and synthesized new perylene derivative containing 2-(naphthalen-2-yl)thiophene functionalized with alkyl end capping units (P1T) by Suzuki coupling reaction. The alkyl substituted end capping units provide enhanced solubility of P1T derivative in theorganic solvents such as chloroform and dimethylchloride at room temperature. The synthesized perylene derivative (P1T) was characterized by the elemental analysis, 1H-NMR, FT-IR. The thermal and photophysical properties of perylene derivative (P1T) was also studiedusing thermalgravimetric analysis (TGA), cyclic-voltametry (CV), UV-Vis absorption and photoluminescence (PL) studies. These results will be presented in detail. Solution processed OTFTs (Top contact) based on spin-coated PNDTT as an active layer showed the higher field effect hole mobility of 0.002 cm2 V-1S-1, on/off ratio of 102, and the threshold voltage atalmost -3 V.

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Synthesis of monodispersed noble metal nanoparticles using organic capping agent in aqueous solution

윤성수, 박원철

서울대 융합과학기술대학원 나노융합학과

For the unique antibacterial properties of the silver nanoparticles, a lot of applications grew up and it is a point of view to produce monodispersed silver nanoparticles. Most of people, who synthesize silver nanoparticles by reduction of $AgNO_3$ using $NaBH_4$, encountered the problem of aggregation and uniformity. The simple way to get well-dispersed silver nanoparticles is still required. Here we investigated the synthesis of silver nanoparticles using organic capping agent such as the triblock pluronic copolymer. TEM(Transmission Electron Microscopy) images show that the triblock pluronic copolymer is so useful as to prevent the aggregation of silver nanoparticles. In addition, the as-prepared silver nanoparticles can be used as seed materials of synthesizing the uniform gold nano-structured particles. XRD(X-Ray Diffraction) was used to analyze the element of gold nanoparticles.

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Templated porous gold nanomaterials by multisegmented alloying-dealloying process

이희옥, 채원식

한국기초과학지원연구원 강릉센터

Noble metal nanostructures have attracted significant attention because of their use in various applications such as catalysis, optics, electronics, chemical sensing, actuators, fuel cells, and microfluidics. In this study, we used gold and silver mixture solution as well as silver solution for pulsed electrodeposition through multistep deposition processes. Alternative deposition of silver and gold-silver alloy segment into the pores of anodic aluminum oxide membrane and subsequent silver etching resulted in enhanced yield of porous gold nanorods with a controlled dimension. The resulting porous gold nanorods would be an efficient 'hot-spot' platform for molecular sensing application.

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Solar energy conversion by the regular arrays of TiO2 nanotubes conducting 4-mercaptobenzoic-acid-linked with CdS/CdSSe quantum dots

박수정, *이성훈

*서울대 나노융합학과 *서울대 화학부*

The regularly ordered anodic titanium oxide (TiO_2) nanotubes are fabricated by electrochemical methods. Their absorption lies in the UV region of the solar spectrum. We need to extend the absorption spectrum to a visible range to enhance solar energy conversion efficiency. As one of the strategies, we attach conducting 4-mercaptobenzoic-acid or its derivatives-functionalized CdS (2.25eV) or CdSSe quantum dots to the regular arrays of titania nanotubes. We investigated solar energy conversion by the regular arrays of TiO_2 nanotubes conducting 4-mercaptobenzoic-acid-linked with CdS/CdSSe quantum dots and observed enhanced photocurrents under AM 1.5 G at 100mW/cm^2 illumination.

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Effects of Polyaniline Additive in Solvent-Free Ionic Liquid Electrolyte for Dye-Sensitized Solar Cell

이재관

호서대

The success of the dye-sensitized photoelectrochemical cell developed by Grätzel and co-workers[1] helped to reinvigorate the search for alternatives to traditional semiconductor photovoltaics in the early 1990s. The enormous efforts for the non-volatile electrolytes such as solvent-free ionic liquids (ILs) and the quasi-solid-state electrolytes with polymer and gelators such as organic and inorganic materials have focused on improving the device performances and stabilities though developments of efficient materials to overcome this problem. [3-7] Among them, solvent-free IL electrolytes has been extensively demonstrated with attractive advantages regarding thermal stability, non-flammability, and high ionic conductivity to realizing commercial production as well as to realizing flexible device, in which molecular solvent may be strongly imposed restriction due to their permeability into plastic substrate. Recently, the respectable efficiency of over 5% was obtained from the photovoltaic cell composed with the amphiphilic ruthenium dye, cis-RuLL'(SCN)2 (L = 4,4'-dicarboxylic acid-2,2'-bipyridine, L' = 4,4'-dinonyl-2,2'-bypyridine) (Z907), and 1-methyl-3-propylimidazolium iodide (PMI-I). And an outstanding achievement has been reported by Grätzel et al. with providing a promising efficiency of over 8% by using eutectic melt-based IL electrolytes. And an incorporating of some additives in solvent-free IL electrolytes has exhibited the enhanced performance of device. In this perspective, we have also attempted new approaches to improve the ion transporting properties in solvent-free IL electrolytes by conjugated polymer additive. We herein present the effects of polyaniline additive in solvent-free IL electrolyte for dye-sensitized solar cell.

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Cytotoxic Potential of Tellurium Nanowires in Fibroblast Cells

Mahto Sanjeev Kumar, 강미선, 김진권, 이석우

공주대 화학과

In this presentation, we demonstrate the cytotoxic potential of Te nanowires in BALB/3T3 fibroblast cells. Te nanowires were synthesized through an aqueous phase surfactant assisted method. Toxicological experiments such as morphological changes, MTT assay, DAPI staining and estimation of intracellular ROS were carried out to investigate the cytotoxic potential of Te nanowires. Te nanowires were found to be cytotoxic at all the concentrations tested in a dose-dependent manner. TEM images revealed that the necrosis was the basic pattern of cell death, which might have caused by the formation of toxic moieties of tellurium, released from nanowire structures, in the bioenvironment. Thus, these observations suggest that Te nanomaterials may pose potential risks to environmental and human health.

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Synthesis of Graphene-Based Silica Nanosheets with Tunable Dimension

남보라, *이하진, *최원산

*충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터*

Graphene, a single layer of sp^2-bonded carbon atoms, has drawn tremendous scientific interest for its extremely high mobility and ballistic transport of electrons. The unique properties of graphene make it an ideal candidate for many applications, such as field-effect transistors, sensors, transparent conducting electrodes, field emitters and supercapacitors.Two dimensional nanosheets or nanoplates have become ideal building blocks for the fabrication of nanoscale devices and structures due to their extremely high anisotropy and a thickness of nanometer scale. Much effort has been focused on controlling dimension of 2D nanosheets to tune unique properties produced from dimensional characteristics. However, a general method to synthesize 2D nanosheets with controllable thickness has been still lacking. Herein we demonstrate the synthesis of silica nanosheets with tunable thickness based on polymer-coated graphene. We used polymer-coated graphene nanosheets (GNSs) as templates for synthesizing silica nanosheets. Polymer-coated GNSs were obtained by reducing exfoliated graphite oxide in the presence of poly(sodium 4-styrenesulfonate) (PSS) and poly(allylamine hydrochloride) (PAH). The utilization of polyelectrolytes not only effectively solves the aggregation problems between graphenes, but also provides the molecular template for controlled nucleation and growth of silica on the surface of GNSs. By this means, 2D sandwich-like graphene-based silica nanosheets can be formed. Silica nanosheets were obtained after calcination of silica/PEM-coated graphene and their thickness were easily controlled by varying reaction conditions. As-prepared silica nanosheets showed smooth surface and free-standing structure with size of several micrometers. A facile route for silica nanosheets with tunable dimension described here could be utilized to further explore functional 2D nanomaterials with applications in catalysis, sensors, supercapacitors, batteries, and fuel cells [1].References [1] Shubin Yang, Xinliang

Feng,* Long Wang, Kun Tang, Joachim Maier, and Klaus Mullen*. Angew. Chem. Int. Ed. 49, (2010) 4795 –4799

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Chemical Reactors for Polymer Nanoparticles with Controllable Shape; Polymer Core-in-SiO_2 Shell Structures for Synthesizing Nanomaterials with Tailored Properties

고혜아, *이하진, *최원산

*충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터*

The fabrication of well-defined structures in the submicrometer ranges has attracted increasing research interest in recent years. Synthesis of nano/microsized hollow spheres with empty interior, in particular, has been one of the most active research areas due to their technical importance in a variety of applications, including drug delivery carriers, catalyst carriers, building blocks for photonic crystals, and nanocapsules for hydrogen storage. Such hollow spheres can be used as chemical reactors for nanomaterials with unique properties as well. Materials that are synthesized within these spatially confined containers often show unique properties that cannot be produced through synthesis in a bulk space. Herein we present specially designed capsule microreactors for synthesizing polymer nanoparticles with controllable shape which is not observed in bulk. Overall shape is hollow spheres with a movable polymer core, referred to as a core-in-shell particle. These core-in-shell particles can be further utilized as templates for synthesizing tailored nanomaterials with controllable properties.

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Mesoporous Structures Generated by Zeolite-Structure-Directing Surfactants

김정남, 조창범, 나경수, 조강희, 정진환, 유룡

KAIST 화학과

Various types of zeolitic materials have been synthesized using surfactant molecules that are functionalized with zeolite structure-directing (SD) groups. These materials exhibit both mesoporosity and crystalline microporous nature of mesopore walls. For example, $C_{22}H_{45}$-$N^+(CH_3)_2$-C_6H_{12}-$N^+(CH_3)_2$-C_6H_{13} can be used to obtain ultrathin MFI zeolite nanosheets with a single-unit-cell-thickness (2.0 nm) along *b*-axis. Depending on the detailed synthesis conditions, the nanosheets can be assembled to irregular aggregation or regular stacking into a multilamellar structure. Surfactants with other-SD head groups can be used to obtain a mesoporous material composed of nanosponge-like disordered network (~4 nm in mesopore diameter, and ~3 nm in wall thickness) of crystalline microporous BEA zeolite, or an MTW zeolite exhibiting nano-needle morphologies. In the synthesis experiment, no conventional SDAs are added. No zeolite structures are generated without these surfactants. Evidently, the surfactant head groups are the zeolite SD agents while the assembly of the tails leads to the generation of mesoporosity or mesoscale morphologies. These zeolites show possibilities as high-performance catalysts in reactions for the production of renewable energy and for the development of green chemical processes. It would therefore be exciting to explore zeolitic materials available via this synthesis route.

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Semiconducting Nanowires for Thermoelectrics: Preparation and Characterization

김하영, 김성진

이화여대 화학과

We synthesized Bi_2Te_3 semiconducting nanowires by electrodeposition and chemical vapor deposition. Bismuth telluride nanowires were deposited electrochemically in the present of each $Bi(NO_3)_3 \cdot 5H_2O$ and TeO_2 in 1.0 M HNO_3 using porous anodic alumina template by pulsed-potential deposition method at room temperature. The pulse potentials for nanowires were selected at more negative potential range than their reduction potential observed from cyclic voltammograms (CVs) and a delay potential was used in no current region between reduction and oxidation potentials of the compound. To obtain dense, highly oriented and single-crystalline nanowires, the growth rate is a critical factor. Also, Bi_2Te_3 nanowires were obtained by a simple evaporation of Bi_2Te_3 powder. Bi_2Te_3 powder were filled in an alumina boat and placed on the inner graphitized quartz tube. This quartz tube is located on the center of the high temperature tube furnace. The furnace was heated to 700ºC under a constant argon gas flowing for deposition. A large amount of Bi_2Te_3 nanowires were grown on the alumina boat placed on the lower temperature part downstream of argon gas flowing without any metal catalyst.The microstructure and morphologies of nanowires were investigated by Powder X-ray diffraction and FE-SEM, HR-TEM. Thermoelectric properties (ZT values) of the nanowires will be discussed.

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Growth of single-crystalline RuO_2 nanowires on the Graphene layer

박지은, 김성진, 김명화

이화여대 화학.나노과학과

Ruthenium oxide(RuO_2) is an attractive electrical contact material, and displays good thermal stability up to 800℃. Moreover hydrous RuO_2 could be used in fuel cells and supercapacitors. And two-dimensional sheet of sp2-hybridized carbon, graphene has inspired research in many directions, due to its outstanding properties. In this study, single-crystalline RuO_2 nanowires were successfully grown on the graphene layer via a physical vapor transport. Graphene was used as the highly effective catalyst in our growth process of the NWs. The control of the sizes(width and length) of the RuO_2 NWs was achieved by adjusting the growth conditions such as flow rate, growth time, and oxygen content. And we could obtain RuO_2 NWs with high density and high crystallinity on the graphene layer. The structure and morphology of RuO_2 NWs were then investigated by X-ray diffraction, Raman Spectroscopy, SEM and HR-TEM.

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Oxygen-defect Tin Oxide Nanostructures : Characterization and Modification

김솔, 김성진

이화여대 화학과

N-type wide band gap(E_g=3.6 eV at 300 K), low resistivity(10^{-4}~10^{-6} Ωcm) and high Li ion storage capacity(781 mAh/g) make tin oxide be attracted great interest recently. These properties make them be important applications as gas sensor, transparent conductor, lithium ion battery and nanoelectronic device and so on. Controlled thermal evaporation growth (TEG) allows the achievement of wide band-gap rutile SnO_{2-x} n-type semiconductor nanostructures with uniform composition and structural perfection. The growth morphologies of various nanostructures are investigated via TEM, SEM and XRD analysis. The prepared SnO_{2-x} nanowires were typically 50 nm~500 nm in diameter and about tens of micrometers in length. The surface of single-crystalline SnO_{2-x} nanowires were further modified with noble metal nanoparticles through self-assemblies with polymers. Poly(vinylpyrrolidone) as a stabilizer plays a key role in loading metal nanoparticles onto the surfaces of SnO_{2-x} nanowires. Sensing performance and other properties of modified SnO_{2-x} nanostructures are also discussed.

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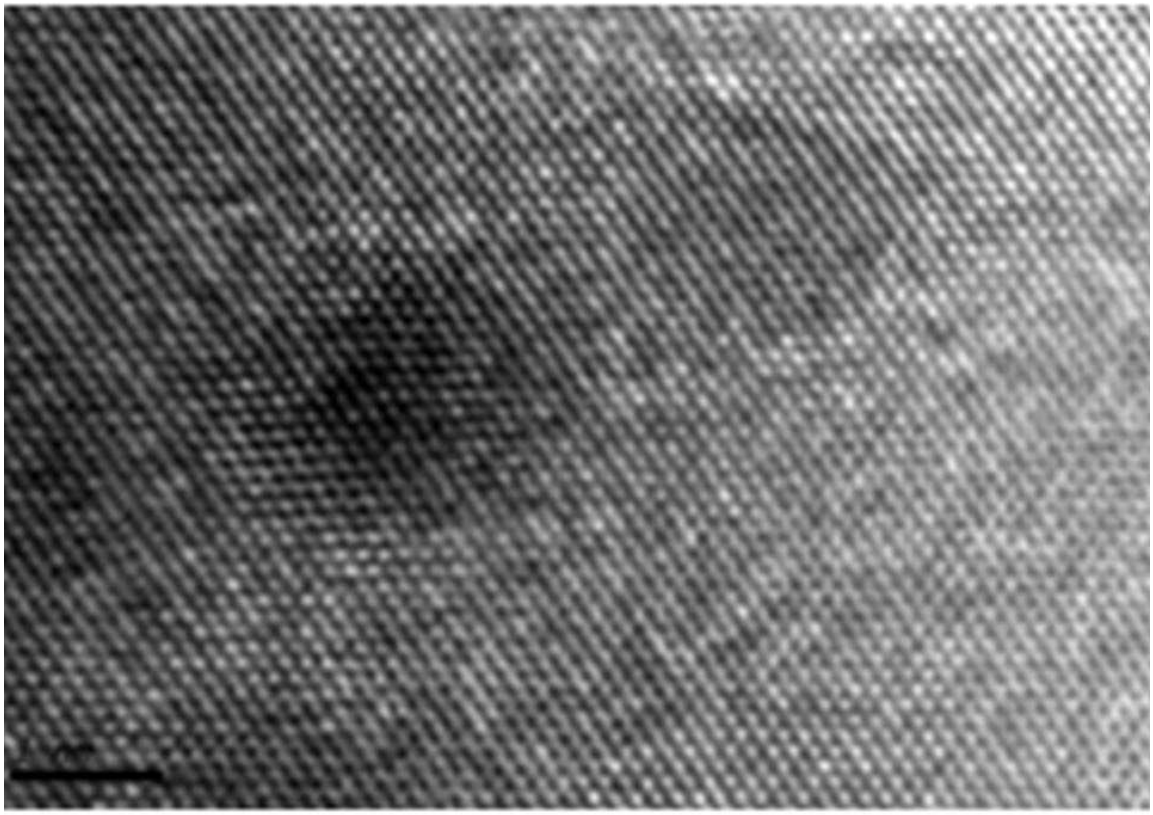
Properties and microstructures of In2Te3 prepared by insertion of Bi2Se3 nanoparticles

김희진, 한미경, *김성진

*이화여대 화학나노과학부 *이화여대 화학과*

The thermoelectric device ability is measured by figure of merit (ZT). ZT is given by ZT=S2σT /κ (where σ is the electrical conductivity, S the thermo power, and κ is the thermal conductivity)For several decades, the ZT of the thermoelectric materials have been less than 1. Current research results often are reported ZT>2 due to quantum confinement effect.We studied thermoelectric properties of In2Te3 prepared by insertion of Bi2Te3 nanoparticles. Bi2Se3 nanoparticles were prepared by solvothermal synthesis.The thermal conductivity and the electrical conductivity decrease with increasing Bi2Se3 nanoparticles contents. The phonons and electrons would be scattered by Bi2Se3 nanoparticles depending on their contents, size. The contents and sizes of Bi2Se3 nanoparticles are critical factor for achieving an increase in ZT compare to In2Te3 bulk. An increase in ZT could be achieved for an optimal contents and sizes of Bi2Se3 nanoparticles.Seebeck coefficient and electrical conductivity have been measured by ZEM-3(Ulvac) and the thermoelectric figure merit calculated.The microstructure and morphologies of In2Te3 insertion of the Bi2Te3 nanoparticles were investigated by Powder X-ray diffraction(Rigaku D/MAX X-ray) and HR-TEM(High resolution Transmission electron microscopy, JEOL 2100F).



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Synthesis of Carbamoylmethylphosphineoxide (CMPO) Analogue for Separation of a Therapeutic Radioisotope

정순재, 유정원, 유국현

동국대 화학과

The separation of radioisotope is crucial for the preparation of therapeutic and tracking radiopharmaceuticals because the radiochemical yield depends on the purity of radioisotope. In this study, we reported the separation of this rare radioactive metal which is effective CMPO derivatives, has been investigated. Present study includes the synthesis of modified ordered mesoporous silicate materials for the effective purification of radioactive CMPO analogue *N*-aminopropyl-*N*-isopropylcarbamoylmethyl)ethoxy phenyl phosphine oxide. The *N*-aminopropyl-*N*-isopropylcarbamoylmethyl)ethoxy phenyl phosphine oxide was prepared starting from 3-bromopropylamine in five steps with approximately 11% overall yield.

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Gold nanoparticle array processing on amino-functional microtemplates fabricated by using vacuum ultra-violet lithography

J. H. Yang, Y. J. Kim, T. Ichii, K. Murase, H. Sugimura

Kyoto University, Japan

Driven by the increasing need for faster and more powerful electronics, research interests have been activated to fabricate new generation electronic or optical devices, which are based on a quantum mechanism. Nanoparticles are hopefully the ideal candidates as building blocks for the new generation device by electrical properties. However, the potential utilization of these nanoparticles requires attaching them onto solid surface, precisely controlling their size and position and electrically connecting them as well. Especially, functionalization of quartz surface has attracted much attention in view of their optoelectronic application by high optical transparency. Here, we demonstrate the arrangement of gold nanoparticles (AuNPs) on quartz substrates with micropatterns. The chemical affinity for immobilizing AuNPs on quartz is provided using 3-aminopropyltrimethoxysilane self-assembled monolayer (APS-SAM). Micropatterns of APS-SAM are fabricated by vacuum ultra-violet (VUV) lithography. The immobilized AuNPs density depending on the micropatterns is studied. Features of area-selectively immobilized AuNPs 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 VUV-irradiated region where the APS-SAM had been removed. In addition, we found that the density of the AuNPs on the boundary of the region where the APS-SAM remained was higher than that of the center part of the region at the initial stage of the immersion. This might be explained the diffusion of AuNPs specific to the boundary regions.

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Templated fabrication and electrochemical characteristics of porous gold photonic crystals

함성경, *채원식, 정진승

*강릉대 화학과 *한국기초과학지원연구원 강릉센터*

Three-dimensional (3D) porous gold photonic crystals were fabricated by a templating route, and were subjected to evaluate their electrochemical properties. A series of casting techniques allowed the polystyrene opal to be replaced with the target bimodal porous gold materials. Silica inverse opal could be simply fabricated by infiltrating silica precursor into the voids of an polystyrene opal template, followed by the removal of the polystyrene colloidal template. Electrochemical deposition of AuAg alloy or Au into a silica inverse opal template and etching of silver after removal of the silica template resulted in 3D porous gold photonic crystals which consisted of interstitial macropores among nanoporous gold spheres. Such the bimodal porosity is experimentally proven to be very useful for enhancing electrochemical reaction rate and accessibility to whole active area inside the 3D porous gold.

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Phthalocyanine Nanoball and Their Application

백강균, Raghunandan Hota, 윤경원, 김영국, 정현태, 박경민, *강주석, *구길호, *박찬경, **배수미, **안웅식, 김기문

*포항공과대 지능초분자 연구단, WCU 첨단재료과학부, 화학과, 시스템생명공학부 *Department of Materials Science & Engineering, POSTECH **Department of Obstetrics and Gynecology, The Catholic University of Korea*

Here we present a one-pot, direct synthesis of novel photosensitive phthalocyanine nanoballs through thiol-ene click chemistry without using any template preorganized structure. Scanning electron microscopy and transmission electron microscopy studies revealed that the nanoball has a spherical shape (average diameter of 210 ± 70 nm) and hollow structure. Furthermore we have utilized the nanoball as a photosensitizer for photodynamic therapy in vitro and in vivo to suppress the tumor growth efficiently. Details of the synthesis of phthalocyanine nanoball and its application in photodynamic therapy will be presented.

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Free-standing, Single-monomer-thick, Two-dimensional Polymers

백강균, 윤경원, 김영국, *김동우, **구길호, **박찬경, ***성봉준, 김기문

*포항공과대 WCU 첨단재료과학부, 화학과, 지능초분자연구단 *CSS, Department of Chemistry, WCU-AMS, POSTECH **Department of Materials Science and Engineering, POSTECH ***서강대 화학과*

Two-dimensional (2D) polymers are expected to have many interesting properties and applications. Although numerous approaches have been reported over the last two decades, the synthesis of covalently bonded, single-monomer-thick 2D polymers with a long-range ordered internal structure has yet to be achieved. Here we present the direct synthesis of free-standing 2D polymers made of host molecules without any templates. The thiol-ene "Click" reaction of allyloxycucurbit[6]uril, a rigid, disk-shaped host molecule with polymerizable allyloxy groups at the periphery, and ethanedithiol in DMA directly produced free-standing 2D polymers. The resulting polymers have been characterized by various techniques including AFM, SEM and TEM. In addition, the embedded molecular cavities of 2D polymers can form strong host-guest complexes with spermine conjugates, which allow us to investigate the internal structure of the 2D polymers.

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A Simple Preparation Method of Photoanode on Flexible Plastic Substrate in Dye-Sensitized Solar Cell

권도훈, 윤용태, 김영일

부경대 화학과

In order to get cost-low flexible dye-sensitized solar cells several attempts such as electrophoresis and microwave irradiation et al have been made to prepare a nanoporous semiconductor film on flexible substrate without high temperature heat treatment. Here we report a simple method of preparing nanoporous TiO2 film on PET/ITO substrate. Titanium alkoxide sol mixed with TiO2 nanopowder without any other stabilizer and subsequent heat treatment at low temperature gave a stable and tightly bound nanoporous TiO2 film on PET/ITO substrate. The prepared TiO2 photoanode was characterized and its performance was tested in an assembled dye-sensitized solar cell.

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A Facile Synthesis Method for Silver Nanoparticle-Polymer Composites and Their Electrically Bistable Properties for Thin-Film Devices

김성호, 지용성, *이탁희, **K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,PIMS **광주과학기술원 신소재공학과,나노바이오전자재료공학과*

Silver nanoparticles have been used for a long time and recently various methods have been additionally developed for their production. Here we report a facile method for the synthesis of silver nanoparticles, in which a polyimide is used for their size control. The synthesis is performed at room temperature without light source and without surfactants to direct the anisotropic growth of the nanoparticles. The formation of the nanoparticles was studied by UV-visible spectroscopy, and transmission electron microscopy. In addition, the bistable resistance state performance was measured for organic-based devices using these polymer-nanocomposite films.

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Nanoencapsulation of Paclitaxel Using Supramacromolecule for Enhanced Cytotoxic Activity

Prasad Rao.J, 이연주, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*

Nanoencapsulation of anti-cancer drugs with the aid of nanoscience and supramolecular chemistry can open up new administration routes for the treatment of cancer. In this context, cyclodextrin offers a wide spectrum of opportunities. In this report, we present the encapsulation of paclitaxel using cyclodextrin-based supramacromolecular nanostructures. It has been found that the encapsulation depends upon the shape and size of the supramacromolecular structures. The supramacrolecular drug complexes were analyzed by FT-IR- and NMR-spectroscopy. The thermal behavior of the complexes was monitored by DSC. The presence and content of the drug in the complexes has been confirmed from XRD and TGA measurements. The visual evidence of the complexes is provided by the TEM images. Interestingly, the supramacrolecular drug complexes exhibited an improved cytotoxic activity against the breast cancer cell lines (MCF-7).

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Enhanced CO_2 Sorption Capacity of Polyethyleneimine-impregnated MSU-J and MSU-F Silica Composites

김미지, *박인

*연세대 화공생명공학과 *한국생산기술연구원 패키징기술지원센터*

Mesoporous MSU-J (pore volume 1.47cm^3/g) and MSU-F (pore volume 2.04cm^3/g) silicas impregnated with polyethyleneimine (PEI) were used for carbon dioxide sorbents. The PEI-impregnated MSU-J (PEI_MSU-J) and MSU-F (PEI_MSU-F) silicas exhibited highly improved CO_2 adsorption capacity compared to other mesostructured silicas (HMS, SBA-15, and MCM-41). In case of 50wt% PEI_MSU-J and PEI_MSU-F PEI did not fill pores due to high pore volumes (>1cm^3/g) of the silicas. The remaining pore volume affords CO_2 molecules to access to internal amine groups of the PEI. The pores of HMS, SBA-15 and MCM-41 silicas (<1cm^3/g) were filled with PEI chains at 50wt% loading as determined by N_2 adsorption-desorption isotherm analysis.

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Synthesis of flower-shaped silver colloids using pulsed proton beam

송재희, *한상우

*순천대 화학과 *KAIST 화학과*

A new solution phase method is presented for the synthesis of “flower-like” silver nanomaterials using pulsed proton beam irradiation process at room temperature. It was observed that the morphology of the prepared silver crystals was easily controlled by the exposure number of pulsed proton beam. The synthesized flower-like silver nanocrystals exhibited excellent surface enhanced Raman scattering (SERS) signals, which were attributed to the rough microstructures on the surface of the synthesized Ag crystals.

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Effect of organic synthesis of structure directing agent, N1-hexyl-N1,N1,N6,N6-tetramethyl-N6-octadecylhexane-1,6-diaminium and its anion exchange level for lamellar zeolitic material

신혜선

전남대 신화학소재공학과

Recently, lamellar zeolitic material have drawn much attention due to unique properties of structure and the resulting catalysis such as extended life compared to conventional catalytic material. For the synthesis of the lamellar zeolitic material, the diaminium compound is functionalized with short and long alkyl chains at the end of both sides. The functionalized diaminium compound can be obtained two subsequent alkylation of tertiary amine using different alkyl halides. In addition, the level of anion exchange determines whether multi- or uni-lamellar zeolitic material can be obtained. In this respect, we modified the synthesis condition of the functionalized diaminium compound to obtain the SDA for the formation of lamellar zeolitic material. Each fraction of the diaminium compound containing difference alkyl groups was analyzed with HPLC. Using the functionalized diaminium compound with different anion exchange levels, the lamellar zeolitic material was obtained readily. The resulting surface properties of the lamellar zeolitic material were characteristics of mesoporous zeolitic material of which the IZC code was MFI.

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Post-synthetic modification of open metal site in metal-organic mesoporous materials

박혜란, Dybtsev N. Danil

포항공과대 첨단재료과학부

Post-synthetic modification (PSM) of metal-organic porous materials (MOPMs) is chemical derivatization of MOFs after their formation involving covalent or coordination bond formation with the framework. The potential advantages of the PSM include the modifications of a given MOPM structure with different reagents thereby generating a large number of topologically identical, but functionally diverse MOPMs. This work represents the post-synthetic modification of a series of mesoporous MOPMs, such as chromium(Ⅲ) trimesiate (MIL-100) and chromium(Ⅲ) terephthalate (MIL-101) by pyridine derivatives through coordinatively unsaturated open metal sites. Such PSM will change the diameter of porous channels, the affinity of pores toward certain guest molecules and enhance the selectivity of sorption. The synthesized materials are characterized by powder X-ray diffraction, TGA, FT-IR spectra, UV reflectance spectra, XPS and gas sorption isotherms.

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Template synthesis of novel rattle-type CuO spheres and its application as anode in lithium secondary batteries

주정훈, 류성현, 류광선

울산대 화학과

Rattle-type hollow structures refer to hollow shells with a solid particle core and interstitial hollow space in between. Owing to their unique structure, rattle-type nanoarchitectures are receiving increasing attention because of their many potential applications, for example, as nanoreactors and nanocontainer.For high-performance LIBs, The improvement of the electrochemical performance brought about by the employment of hollow micro-/nanostructures can in reality be explained in terms of multiple factors. First, the cavities in the hollow structure may provide extra space for the storage of lithium ions, which is beneficial for enhancing specific capacity of the battery. Second, the hollow structure is often associated with larger surface area and reduced effective diffusion distance for lithium ions, leading to better rate capabilities. Third, the void space in hollow structures buffers against the local volume change during lithium insertion–deinsertion and is able to alleviate the problem of pulverization and aggregation of the electrode material, hence improving the cycling performance.We synthesized the CuO with novel rattle-type structure. The rattle-type structured CuO particles were prepared by the soft templates. We studied the physical properties of this material with XRD, SEM, and TEM etc. The electrochemical properties of this material as anode materials were analyzed by CV curves, charge-discharge capacity, and cycling performance. We expect that the CuO induced by rattle-type structure will improve the electrochemical cycling ability, capacity retention, and rate capability as anode in lithium secondary battery.

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Synthesis and properties of polymer based dialkylated-terthiophene for OTFT

강소희, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

Organic semiconducting molecules were very attractive for the fabrication of organic thin film transistors (OTFTs) in various molecular electronics applications, such as flexible display, smart card, RFID tag, and electronic paper.Lately, the researchers have made solution-processable materials based on polythiophenes, because they have good electrical conductivity as p-type semiconductors. In particular, poly(3-alkylthiophene) derivatives have been intensively studied. The head-to-tail regioregularity of poly(3-hexylthiophene)s assemble into a highly ordered architecture (large crystalline domain), and possess an extended planar π-stacked system, resulting in high charge-carrier mobilities.In this research, we designed and synthesized the new polymer which is composed of dialkylated-terthiophene. And the characterization of the polymer will be discussed.

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Role of Multi-Quaternary Ammonium Groups in Surfactant Molecules as Structure-Directing Agents for MFI Zeolite Nanosheets

조창범, 유도애, 정진환, 유룡, *Dongdong Xu, *Shunai Che

*KAIST 화학과 *School of Chemistry and Chemical Engineering, Shanghai Jiaotong University*

Various surfactants containing one or more quaternary ammonium groups have been investigated as structure-directing agents for zeolite MFI in aqueous gel compositions that do not lead to zeolite crystallization without such surfactants. No conventional zeolite structure-directing agents such as tetrapropylammonium bromide and hydroxide were included in the synthesis compositions. The synthesis conditions were also controlled so that zeolite could not be generated by sodium ions. The present study shows that at least two ammonium groups need to be bonded in a row through hexamethylene bridges to a surfactant tail, e.g., $C_{22}H_{45}$-$N^+(CH_3)_2$-C_6H_{12}-$N^+(CH_3)_2$-C_6H_{13}. Ultrathin zeolite nanosheets were generated by the surfactant head groups whereas the surfactant tails were longer than a decyl group. The thickness of the zeolite nanosheets was consistently increased by the number of quaternary ammonium groups. Bulk zeolite crystals were generated instead of nanosheets where the surfactant tails were shorter than or equal to octyl. Other design factors for surfactant have also been investigated, such as substitution of methyl to higher alkyl groups, and insertion of quaternary ammonium groups between two long alkyl chains. Structures of the resultant zeolitic nano-architectures have been characterized by X-ray powder diffraction, N_2 adsorption and transmission electron microscopy. This synthesis result is provided to shed light on the structure-directing role of the surfactant molecules.

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Interfacial interaction induced mesophase orientation in different confinement dimensions

김은미, 채원식

한국기초과학지원연구원 강릉센터

Mesophased silica materials have been typically developed through surfactant guided soft-templating route using lyotropic mixtures consisting of block copolymers and inorganic precursors. In this study, we evaluate the confinement effects of a lyotropic mixture within a 1D and a 2D confining environment. Within a given confinement energy, i.e., a given film thickness and a given lateral width depending on 1D and 2D confinement, respectively, the confined guest mesophased system suffers strong interfacial interaction with confining host surfaces where may have hydrophilic or hydrophobic chemistry, therefore, it is experimentally proven that a threshold energy is required to have an optimal orientation of the confined system. The resulting mesophased silica nanoporous materials with an engineered internal pore orientation would be very useful for the fabrication of unique structured nanomaterials as templates.

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High performance CNT/Si composite anode materials forlithium ion batteries

양대수, *김민식, *김정호, *유종성

*고려대 신소재화학 *고려대 신소재화학과*

Silicon and silicon containing compounds are attractive anode materials for lithium batteries because oftheir low electrochemical potential vs. lithium and high theoretical capacities. In this work, silicon coating on the multiwall carbon nanotubu using the pyrolysis of silica was found to be crucial for making good electronic contact to the material. and investigated with scanning electron microscopy, transmission electron microscopy, X-ray diffraction, and electrochemical experiments.The CNT@Si nanocables show excellent rate capability and cycling performance compared with both pureCNTand pure TiO2 when used as anode materials for lithium-ion batteries (LIBs).

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Separation of Single-walled carbon nanotubes: Effect of electron-donating and electron-withdrawing substituents on Agarose bead

박용선, 장형석, *경산, 이윤식

*서울대 화학생물공학부 *서울대*

Single-walled carbon nanotubes(SWNTs) have a great potential to be used in various nano-application fields due to their unique electronic and mechanical properties. However, the coexistence of metallic and semiconducting SWNTs in the commercial one is preventing their wide applications.Recently, a novel and simple method using agarose bead to selectively separate semiconducting nanotubes from metallic nanotubes was reported. In our study, we try to demonstrate that there exist critical interactions between agarose bead and SWNTs by employing various electron-withdrawing and electron-donating groups on the agarose bead. Effective separation was verified by absorption and Raman spectroscopic analysis.

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Effects of Polyelectrolyte Intercalation on the Chemical and Electrochemical Properties of Layered Manganese Oxide

이경민, *김태우, **황성주

*이화여대 화학나노과학과 *이화여대 지능형 나노바이오소재 연구센터 **이화여대 화학·나노과학과*

We have investigated the effects of polyelectrolyte intercalation on the chemical and electrochemical properties of layered manganese oxide. The intercalative nanohybrids of layered manganese oxide and several polyelectrolytes such as polyethyleneimine (PEI), poly(diallydimethyl ammonium) chloride (PDDA), and poly(allylamine hydrochloride) (PAH), were synthesized by self-assembly between negatively charged MnO_2 nanosheets and polycations. Powder X-ray diffraction analysis clearly demonstrated that the obtained samples show the well-ordered intercalation structure with expanded basal spacings (ca. d_{001}=1.3~2.7 nm) that depend on the chemical nature of the guest polyelectrolytes. The formation of the intercalative nanohybrids was cross-confirmed by FT-IR analyses showing characteristic IR bands corresponding to the stretching and bending modes of $-CH_2-$and$-CN-$ units. N_2 adsorption-desorption isotherm analysis indicated that the PEI-layered MnO_2 nanohybrid showed a larger surface area than the other nanohybrids and the pristine $K_{0.45}MnO_2$. According to Mn K-edge X-ray absorption spectroscopy, the PEI-layered MnO_2 nanohybrid possessed a lower Mn oxidation state compared with the others, which is due to the presence of Lewis basic amine groups in the PEI. The obtained hybrid materials were tested as electrode material for supercapacitor. Based on the obtained results, we will discuss the effect of polyelectrolyte intercalation on the electrochemical activity of layered manganese oxide in detail.

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Two Dimensional Nanosheets of Spinel-Structured Li4Ti5O12 Applicable for Lithium Intercalation Electrode

한송이, *김인영, *황성주

*이화여대 *이화여대 화학·나노과학과*

We have successfully synthesized spinel-structured $L_4Ti_5O_{12}$ electrode material in the form of two-dimensional (2D) nanosheet. The 2D lithium titanates were synthesized by lithiation for exfoliated nanosheets of layered titanate and the following heat-treatment at elevated temperatures. According to powder X-ray diffraction analysis, the obtained materials show typical Bragg reflections of spinel-structured $L_4Ti_5O_{12}$ (JCPDF-261198). Field emission-scanning electron microscopic analysis clearly showed the 2D nanosheets-like morphology of the present material with the thickness of ~30 nm and the lateral size of several hundred nanometers. From X-ray absorption spectroscopic analyses at Ti K-edge, all the present materials possess tetravalent titanium ions in the spinel lattice. The electrode activity of these materials was examined with the cut-off voltage of 1.0-2.0 V. The relationship between crystal morphology and electrochemical properties in the obtained spinel $L_4Ti_5O_{12}$ nanosheets will be discussed in detail.

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Cucurbit[6]uril: Organic Molecular Porous Material for Selective Carbon Dioxide Sorption

김용휘, 김현욱, 윤민영, 임소영, *서곤, 김기문

*포항공과대 지능초분자 연구단, WCU 첨단재료과학부, 화학과 *전남대 공업화학과*

The organic molecular porous material (1) obtained by recrystallization of cucurbit[6]uril (CB[6]) from HCl shows a high CO_2 sorption capacity at 298 K, 1 bar. Most interestingly, 1 showed the highest selectivity of CO_2 over CO among the known porous materials so far. The remarkable selectivity of CO_2 may be attributed to the exceptionally high enthalpy of adsorption (33.0 kJ/mol). X-ray crystal structure analysis of CO_2 adsorbed 1 revealed that three independent CO_2 sorption sites, two in the 1D channels (A and B), one in molecular cavities (C). The CO_2 molecules adsorbed at sorption sites A near the wall of the 1D channels, interact with 1 through hydrogen bonding, and at the same time with those at sites B mainly through quadrupole-quadrupole interaction in a T-shaped arrangement. Interestingly, two CO_2 molecules are included in the CB[6] cavity (sites C), interacting not only with the carbonyl groups of CB[6] but also with each other in a slipped-parallel geometry. The exceptionally selective CO_2 sorption properties of 1 may find useful applications in the pressure swing adsorption (PSA) process for CO_2 separation. Details of the work will be presented.

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Growth of wurtzite ZnO-cubic $Zn_{1-x}Cd_xSe$ core-shell nanocable arrays for photoelectrochemical cell

명윤, 강준하, 박정희

고려대 소재화학과

High-density wurtzite ZnO-cubic $Zn_{1-x}Cd_xSe$ core-shell nanocable arrays were synthesized on large-area Ni substrates. The outer layers were deposited on the pre-grown vertically-aligned ZnO nanowire arrays using the chemical vapor transport method. Their shell alloy composition controlled by growth temperature and reaction time. The structure and composition of nanocables were analyzed using X-ray diffraction, X-ray photoelectron spectroscopy, high-resolution transmission electron microscopy ,energy-dispersive X-ray spectroscopy and UV-visible spectroscopy showing the consistent values of Zn and Cd composition. In addition, we were found that the nanowire arrays have good light absorption characteristics and these properties make it suitable for photoelectrochemical cell.

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Porous Nanocomposites of Layered Manganese Oxide Nanosheets and Graphene Nanosheets

이유리, *송민선, **이경민, 황성주

*이화여대 화학·나노과학과 *이화여대 화학.나노과학과 **이화여대 화학나노과학과*

We have successfully synthesized porous nanocomposites composed of layered manganese oxide nanosheets and graphene nanosheets. As precursors, both nanosheets of layered manganese oxide and graphene oxide were prepared in the form of well-dispersed colloidal suspension. After mixing both the suspensions, the resulting mixed colloids were freeze-dried and heated at elevated temperatures. According to the powder X-ray diffraction analysis, the resulting nanocomposites show amorphous structures, indicating the formation of homogeneous and disordered mixture without any phase separation. The reduction of graphene oxide to graphene upon the heat-treatment was confirmed by the disappearance of graphene oxide-related peaks, i.e. the vibrations of carboxyl-OH and of C-O stretching. Field emission-scanning electronic microscopy/energy dispersive spectrometry clearly demonstrated the formation of porous structure by the house-of-cards type stacking of layered crystallites and the homogeneous distribution of manganate in the nanocomposite. The expansion of surface area was confirmed by N_2 adsorption-desorption isotherm measurements. In the light of this, we examined the applicability of the obtained nanocomposites as electrode material for supercapacitors by performing cyclic voltammetry with diverse electrolytes. The electrochemical property of the nanocomposite will be discussed in detail.

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Development of York-shell Type Nanoparticles as Surface-enhanced Raman Scattering Probes

강태규, *강호만, **채진주, ***김지영, ****김건성, *****정대홍, 이윤식

*서울대 화학생물공학부 *서울대 협동과정 나노과학기술전공 **서울대 과학교육학과 ***서울대 융합과학기술대학원 ****서울대 사범대 화학교육과 *****서울대 화학교육과*

Surface-enhanced Raman scattering (SERS) has gained a lot of attention as a sensitive analytical tools. It has several advantages that there are large number of Raman tagging compounds, which are lack of photo-bleaching, giving narrow band width with single laser excitation for the detection of multiple labels. In spite of these advantages, SERS probes still need to be improved for stable, enhanced, reproducible, and controllable Raman signals. We have recently reported on several types of SERS tagging materials (SERS dotsTM) composed of silver nanoparticles (NPs) embedded silica nano spheres for various bio-application. Herein, we report the preparation of york-shell type SERS dotsTM by self-templated synthesis of hollow structure via simultaneous core-dissolution and shell-growth process, and the aggregation of silver NPs induced at the core region of SERS dotsTM. This new type SERS probe gives rise to highly reproducible and enhanced Raman signals.

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Synthesis and Characterization of Intercalative TiO_2 Nanoparticle-Graphene Nanohybrid with Improved Photocatalytic Activity

김인영, *김태우, 황성주

*이화여대 화학·나노과학과 *이화여대 지능형 나노바이오소재 연구센터*

We were successful in synthesizing an intercalative TiO_2-graphene nanohybrid system via a reassembling between exfoliated graphene nanosheets and TiO_2 nanoparticles. This intercalative nanohybrid was achieved by an exfoliation-reassembling reaction based on an electrostatic interaction between TiO_2 nanosol particle with positively charged surface and exfoliated graphene nanosheet with negatively charged surface. Powder X-ray diffraction and high resolution-transmission microscopy revealed the formation of intercalation structure composed of well-ordered graphene layers and TiO_2 nanoparticles. According to the N_2 adsorption-desorption isotherm measurement, TiO_2-graphene nanohybrid showed much larger surface area (~366 m^2/g) than that of graphene (~38 m^2/g), underscoring the formation of highly porous structure by the intercalation of titania. Tests of the photocatalytic activity of the nanohybrid clearly demonstrated that this hybrid material is highly active for the photodegradation of organic compound under the irradiation of UV light ($\lambda > 295$ nm). The present reassembling method is quite effective not only in synthesizing novel graphene-based porous materials but also in improving the photocatalytic activity of semiconducting nanoparticles.

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Unusually High Photocatalytic Activity of CdS Quantum Dot-Layered TiO_2 Nanohybrids for Hydrogen Production under Visible Irradiation

김효나, *김태우, **김인영, **황성주

*이화여대 화학·나노과학과 *이화여대 지능형 나노바이오소재 연구센터 **이화여대 화학·나노과학과*

CdS quantum dots (QDs)-layered TiO_2 nanosheet hybrids were synthesized by electrostatic attraction between positively charged CdS QDs and negatively charged exfoliated TiO_2 nanosheet. As a precursor, well-dispersive amine-modified CdS QDs in aqueous solution was prepared by one-pot soft-chemical method. UV-vis spectroscopy, zeta potential measurement and transmission electron microscopy clearly demonstrated the formation of monodisperse positive surface charged (+53 mV) CdS QDs showing the first excitation peak at 370 nm and the uniform particle size of ~2.5 nm. The obtained well-disperse suspension of amine-modified CdS QDs was added dropwise to exfoliated TiO_2 nanosheets colloid. A combinatorial analysis of transmission electron microscopy, selected area electron diffraction, and powder X-ray diffraction clearly demonstrated the formation of CdS′ TiO_2 nanohybrids. According to the powder X-ray diffraction analysis, the resulting CdS QDs-layered TiO_2 nanohybrid exhibited a series of *(00l)* Bragg peaks at low angle region ($2\theta < 10^{o}$′), indicative of the formation of intercalation structure with layer-by-layer ordering. From UV-vis spectroscopy, CdS-TiO_2 nanohybrid showed a distinct change of bandgap energy from 3.5 eV (CdS QDs) to 2.7 eV (CdS-TiO_2 nanohybrids). On the basis of such results, we tested the photocurrent response and photocatalytic performance of the nanohybrids against hydrogen evolved reaction under visible light irradiation.

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Characterization of sulfur containing ordered mesoporous carbons and their application as solid acid catalyst

김진회, 김지만

성균관대 화학과

Ordered mesoporous materials are commonly used in many fields such as adsorbent, chomatography, gas separation, catalysis. Pore size, pore structure, and specific surface area have been regarded as important characteristics of ordered mesoporous materials. And many research groups study in functionalization of ordered mesoporous materials such as silica, carbon and metal oxide. There are two classes of method for surface functionalization by one or two-step modification. One-step method is promoted by precursor which has hetero element in synthesis procedure and two-step approach is post treatment with active gases on prepared material's surface. These materials show enhanced properties that thermal stability, conductivity, fire resistance, sorptivity, and these functional groups are easy to modify to other one. Especially, sulfur containing materials used to heavy metal sorbents, capacitance materials, and solid acid catalyst.

We have chosen one-pot synthesis strategy for fabrication of sulfur containing mesoporous carbon (S-OMC) by nano-casting method with *p*-toluenesulfonic aicd as sulfur containing precursor. According to this method, we fabricate mesoporous carbon which has high specific surface area and heteroatomic functionality. These materials are easy controlled the content of sulfur element in the mesoporous carbons by controlling carbonization temperature. And this synthesis method is less toxic than other synthesis method due to it isn't need to polymerization catalyst such as sulfuric or phosphoric acid.

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Synthesis and Characterization of Selectively Ag coated Nanoparticles Containing Au Disks in the Core

홍순창, *장호영, *조상현, **장민선, 박성호

*성균관대 화학과 *성균관대 에너지과학과 **성균관대 물리.화학융합협동과정*

We present a simple synthetic method for Ag coated nanoparticles containing Au disk in the center. Our synthetic method relies on the synthesis of triangular nanoplate that is followed by selective etching and growth under mild reduction conditions, leading to the formation of Au@Ag nanoparticles. Selective etching of specific facets of triangular nanoplate has led to the Au rounded nanodisks. We used the resulting Au nanodisks as a seed, and the Au core could be coated with Ag. Final shape of Ag coated nanoparticles can be controlled by the presence of iodide ions and amount of Ag ions. Also Au@Ag nanocrystals can be converted into hollow nanostructures made of Au, Pt, and Pd via galvanic replacement reactions

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Gold Nanoprism and Hexagonal Nanoplate Films for Surface-Enhanced Raman Scattering

이두리, 김수진, 이상아, *조성환, 박성호

*성균관대 화학과 *성균관대 에너지과학학과*

In our previous work, we fabricated three-dimensional multilayer films with Au nanorods and nanospheres to investigate the SERS enhancement effect as a function of top layer structure and the nanoparticle packing orders. In this research, we fabricated close packed two-dimensional Au nanoprism and hexagonal nanoplate films by controlling the concentration of linker molecules and temperature of the colloidal solution. Using a method of subsequent transferring such highly ordered film, three-dimensional multilayer films of nanoplates were formed to compare SERS enhancement of each film. We found that nanoprism films show stronger enhancement than hexagonal nanoplate films.

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Optical Properties of Au-Ni Bimetallic Nanorods

김현정, 유상훈, LIULICHUN, *박연주

*성균관대 화학과 *성균관대 에너지과학과*

We report the correlation between multiple modes of localized surface plasmon resonance (LSPR) and the diameters of Au nanorods, and a dependence of optical coupling on relative lengths of Au and Ni building blocks in bimetallic nanorods. The higher mode LSPR of Au nanorods with 60 nm in diameter were obviously observed and compared with that of ones with 80 nm diameter with the same aspect ratios. For two-segment nanorods of Au-Ni with controlled overall length, optical coupling occurred when the lengths of Au moieties were longer than that of the counterpart Ni block. Both observations are conducive to understanding how the dimensions affect the optical outcome and tune output signals of nanorod-based sensors.

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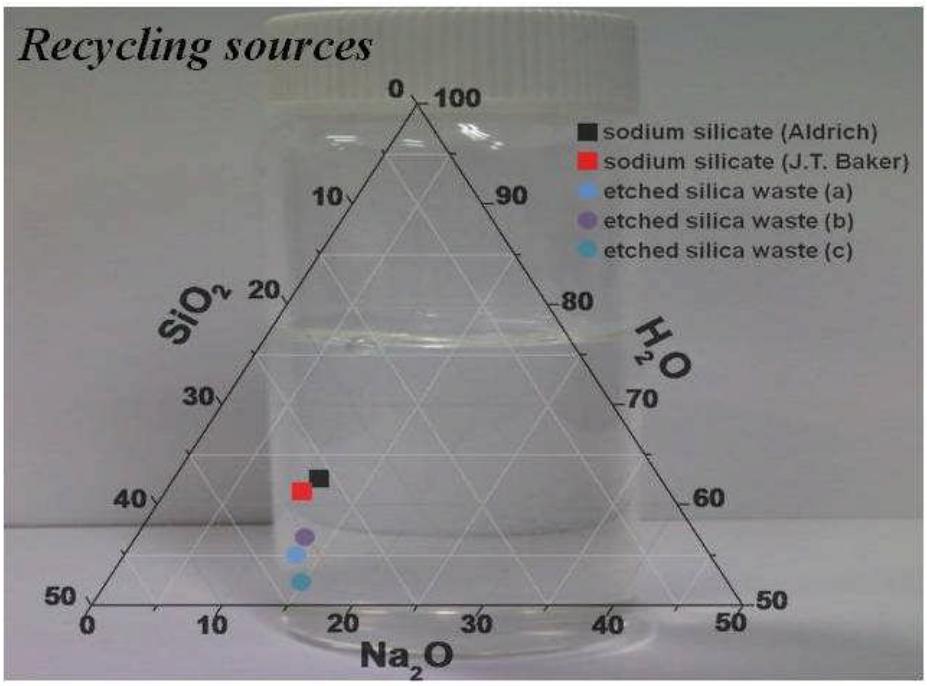
Recycling of a silica template waste into mesoporous materials

김정호, 김민식, *kiran chaudhari, *Nitin Chaudhari, Paul Gouri Sankar, *김민우, *임신묵, **양대수, *송민영, *김윤경, 유종성

*고려대 신소재화학과 *고려대 소재화학과 **고려대 신소재화학*

Recycling of etched silica waste released from nanocasting synthesis of a mesoporous carbon is successfully performed to produce valuable mesoporous silica materials, which can help not only in saving chemicals, but also in decreasing chemical waste for better improvement of our environments. This is a good example of a green chemistry for chemical saving and environmental protection. The silica waste from the colloidal crystal hosts in addition to mesoporous silica host such as SBA-15 investigated in this work can also be examined for recycling. All related works are currently under progress.



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N-Fluorenyl Carbazole Based Conjugated Oligomer for Blue Organic Light Emitting Diodes (OLEDs)

신민기, *장재완, 고혜진, **김윤희, ***권순기

*경상대 고분자공학전공 *경상대 고분자공학과 **경상대 화학과 ***경상대 나노신소재공학부*

Organic light-emitting devieces (OLEDs) have attracted much attention due to their potential applications. For realization of full color flat panel displays, red , green, and blue light emitting materials with sufficient efficiency and good color purity are required. In comparison with red and green light emitting materials, blue light emitting materials show low color purity, thermal stability and lifetime. These problems influence the device lifetime and efficiency. Though carbazole based materials showed good hole transporting properties , low glass transition temperature and high triplet energy, but carbazole based materials were chemically unstable in devices. Fluorene based materials showed high photoluminescent quantum yield, good thermal stability and solubility. In this report, we designed and synthesized BDFC blue emitting materials by yamamoto coupling reaction in order to improve the device efficiency and stability. The photoluminescence (PL) spectrum of BDFC exhibited blue emission at 414 nm in chloroform solution and 409 nm in film. The thermal, photophysical and electroluminescence properties of these materials were characterized and results will be presented in detail.

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Synthesis and Characterization of Alkylthiophene Substituted tetrahydropyrene Derivatives and OTFT Characteristics

고혜진, 신민기, *장재완, **김윤희, ***권순기

*경상대 고분자공학전공 *경상대 고분자공학과 **경상대 화학과 ***경상대 나노신소재공학부*

Organic thin-film transistors(OTFTs) have much attracted interest due to its low-temperature, low-cost, and large-area electronic applications. We reported the new organic thin film transistor (OTFTs), which is composed of a tetrahydropyrene core unit and alkylthiophene on both sides, HHTHT was synthesized Suzuki coupling reaction. The synthesized HHTHT materials were characterized by FT-IR and ^{1}H-NMR and Mass analysis. The thermal properties were determined by thermogravimetry analysis (TGA) and differential scanning calorimetry (DSC). Electrical and optical properties of these oligomers were studied using UV-visible and photoluminescence (PL) studies in solution and film.

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Size and morphology controlled various manganese oxide on silica sphere for core-shell structure

류성현, 주정훈, 류광선

울산대 화학과

The surface coating of nanoparticles with various materials to form core–shell morphologies results in the formation of new materials that can be used in the areas of electrochemical, magnetic, mechanical, thermal, electro-optical, electronics, photonics, and catalysis, etc. Silica coated with other materials is classic materials widely used in many fields of colloid and materials science. The silica core has many merits. First, silica can be easily made controllably in spherical morphology from nano to micron size. If the silica spheres are coated with electrode materials, a kind of core–shell electrode materials with spherical morphology will be obtained, and the size for the electrode materials can be controlled by the silica cores. Secondly, the non-agglomeration, narrow size distribution and perfect spherical shape are many advantages in various application fields.In this study, we studied about silica as a core and manganese oxide as a shell with controlled thickness and morphology. We synthesized silica and silica-manganese oxides with core-shell structures via stöber process and precipitation method. We controlled precursor agent, chelation agent, precipitation agent, and temperature for control thickness of manganese oxide. After that, we carried out the solid solution reaction with lithium source for lithium ion battery cathode materials. We measured the effects of the microstructure and morphology by XRD, FT-IR, FE-SEM, FE-TEM, and BET. We fabricate coin cell for evaluating the electrochemical properties and performance of these materials as cathode materialsAs a result, the various manganese oxides on silica sphere were obtained with a very uniform and spherical character. Also manganese oxides were confirmed with a controlled size and morphology.

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Noval Asymmetric dication synthesis

조원제, 서용성, 박승일, 이진희, 유국현

동국대 화학과

ILs 는 green chemical reagent 및 electrolyte 로서 주목을 받고 있다. 특히 이차전지분야에서 ILs 는 전기 전도도성이 우수하며 비휘발성인 특성으로 인해 전지전해질 대체물질로 그 가치를 인정받고 있다. 본 연구는 전기전도성이 우수하며 동시에 저온 유동성을 확보할 것으로 기대되는 2 가 양이온 ILs 를 합성한다. 그리고 합성된 ILs 는 전기전도도, 저온 상안정성 등에 관한 전기화학적 평가를 통해 고성능 이차전지용 전해질로 사용가능함을 조사하고자 한다.

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Fluoride alkylchain substituted ionic liquids

조원제, 서용성, 박승일, 김대진, 유국현

동국대 화학과

2000 년 후반 들어 급속히 발전하고 있는 ILs 는 green chemical reagent, electrolyte, 윤활유 등과 같은 산업분야에서 꿈의 Solvent 로 주목을 받고 있다. 특히 비휘발성 및 우수한 전기전도성 으로 인해 이차전지분야 그 가치를 높이 평가받고 있다. 본 연구는 대표적 ILs 로 알려진 monocation type ILs 에 열적안정성이 우수할 수 있도록 Fluoride alkylchain 을 Head group 내에 치환한다. Fluoride alkylchain 치환형 ILs 는 전기전도도, 열안정성평가등을 통해 물성평가를 실시한다. 이러한 Fluoride alkylchain 치환 ILs 는 이차전지 및 연료전지분야 전해질분야의 열안정성 개선에 적합한 물질로 기대 된다.

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Crystal structure and ionic conductivity of Li-containing phosphate, $Li_2AlSr_2(PO_4)_3$

김성철, 이미선, *박소정, **윤호섭, 김승주

*아주대 에너지시스템학부 *아주대 응용화학 **아주대 화학과*

New Li-containing phosphate, $Li_2AlSr_2(PO_4)_3$ was synthesized by solid state reaction. It crystallizes in the monoclinic space group $P2_1/n$ (No. 14) with lattice parameters a = 4.945 Å, b = 22.088 Å, c = 8.632 Å, and β = 91.47°. $Li_2AlSr_2(PO_4)_3$ is a layered structure and it have two rigid layers formulated with $2[Al(PO_4)_2]^{3-}$ and their framework is built up from AlO_6 octahedra and tetrahedral PO_4 groups. In the framework, oxygen atoms surrounding the Al atoms are shared with PO_4 tetrahedra while the latter have three bridging oxygens and a terminal one. Impedance analysis was performed to determine the ionic conductivity, the compound exhibits the ionic conductivity of 2.16 x 10^{-4} S/cm at 830 K with an activation energy of 1.03 eV.

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Synthesis of 131I labelled 3-iodo-L-tyrosine grafted Fe3O4@SiO2 Nanocomposite for Simultaneous SPECT and MRI

조원제, 김지원, 이원길, 김영순, 유국현

동국대 화학과

The synthesis of core-shell structure can be achieved by coating or encapsulating them with suitable materials for desired properties. As a tumor imaging agent for SEPCT and MRI, we successfully developed 3-[131I]iodo-L-tyrosine grafted Fe3O4@SiO2 core-shell nanomaterials. Fe3O4 nanoparticle was synthesized through thermal decomposition and Fe3O4@SiO2 was prepared by reverse microemulsion method. After grafting aminopropyltriethoxysilane, L-tyrosine was introduced by amide coupling reaction. Finally, [131I]iodide was labeled on L-tyrosine grafted Fe3O4@SiO2 nanocomposite by aromatic iodination using chloramine-T. The physicochemical characterizations on the nanocomposite have been carried out, along with measurements of its radio-chemicalactivity.

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Metal-free D-π-A Substituted Sensitizers for Dye-sensitized Solar Cells : Synthesis, Properties, and Photovoltaic Performances

김종형, *계광열

*(주)솔라시스 *아주대 화학과*

Novel donor-π-acceptor (D-π-A) dyes, coded as SD-1, SD-2 and SD-3, were designed and synthesized for dye sensitized solar cells. All these dyes comprised the same donor and acceptor units while the oligo thiophene units are introduced as linkers between the donor and acceptor units. The photophysical and electrochemical properties of the dyes were investigated by UV-vis spectrometry and cyclic voltammetry. The dyes were subsequently tested as sensitizers in dye-sensitized solar cells. Photovoltaic performance of device with SD-2 dye showed maximum monochromatic incident photon to current efficiency (IPCE) of 85% and an over all conversion efficiency of 6.2% under full sunlight (AM 1.5G, 100 mW cm-2) irradiation.

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Chemically and Physically Controlled Optical Properties of the $Cd_xZn_{1-x}Se$ Ternary Semiconductor Materials with Highly Ordered Mesostructures

이윤연, *김지만

*성균관대 나노과학기술협동학부 *성균관대 화학과*

Recently, there has been great interest in the synthesis and application of various kinds of nanostructured metal chalcogenide compounds such as ZnX, CdX, PbX, and CuX (X = S, Se, Te). Especially, II-group metal based chalcogenide compounds have been widely investigated in the field of quantum dots, nanodevice fabrication, and energy applications because of their unique chemical and physical properties.Herein, we report on a facile synthetic route to highly ordered mesoporous II-VI binary and II-II-VI ternary semiconductor materials with crystalline frameworks via nano-replication method and their unique optical property studies by UV-visible spectroscopy.

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Room Temperature Synthesis of Nanostructured Manganese Oxides with Various Crystal Structures and Morphologies

성다영, *김인영, **김태우, *황성주

*이화여대 화학나노과학과 *이화여대 화학·나노과학과 **이화여대 지능형 나노바이오소재 연구센터*

The nanostructured δ-, γ-, and α-MnO_2 materials were prepared at room temperature via one-pot oxidation reaction of divalent manganese compounds. Various reactions with many precursors and oxidants were carried out to tailor the crystal structure, morphology, and electrode performance of nanostructured manganese oxides. According to our analysis using powder X-ray diffraction and electron microscopy, treating $MnSO_4$ precursor with persulfate ions at room temperature yields γ-MnO_2 structured manganese oxides whereas the reaction between persulfate ions and MnO precursor and between persulfate and $MnCO_3$ precursor results in the formation of tunnel-structured α-MnO_2 and layered δ-MnO_2 phase, respectively. The persulfate-treatments at room temperature for other manganese compounds that have a higher Mn oxidation state of >+2 do not cause any structural transformation of the precursor phases. The use of other oxidizing agent like H_2O_2 or $NaClO_3$ is not successful in preparing the nanostructured manganese oxides. Scanning electron microscopic analysis clearly demonstrated a 3D nanourchin-type morphology for both the γ-MnO_2 and α-MnO_2 materials and a 2D nanoplate-type morphology for the δ-MnO_2 material. According to electrochemical measurements, the nanostructured manganese oxides showed lithium storage capacity, indicating their potential applicability as electrode materials for lithium secondary batteries.

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Evolutionary Superlattice Structure of $Cu_{1.8}S$ and Cu_2S Nanowires from CdS Nanowires via Gas-Phase Substitution

김한성, 성태광, 장소영, 박정희, *안재평

*고려대 소재화학과 *KIST 산업화지원센터*

Single-crystalline wurtzite CdS nanowires underwent a vapor-phase substitution reaction into a unique superlattice cubic $Cu_{1.8}S$ (digenite) and hexagonal Cu_2S (chalcocite). The $Cu_{1.8}S$ nanowires consisted of the superlattices along the direction, with controlled growth direction ([110], [211], [100], [111]) and superlattice period (1.6 and 1.9 nm). The Cu_2S nanowires also showed a superlattice along the [0001] growth direction, with aperiodicity of 2.7 nm, and could irreversibly convert into the $Cu_{1.8}S$ by electron-beam irradiation.

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Synthesis indium tin oxide(ITO) nanorods and film by RF-magnetron sputter

박재형, 박후근, 도영락

국민대 생명나노화학과

Tin doped-indium oxide nanorods and films were prepared on a glass substrate by RF-magnetron conventional sputtering using an ITO target composed of undoped In_2O_3 (90 wt%):SnO_2 (10 wt%). In order to enhance the optical and electrical properties of an ITO thin film and nanorods, we studied the preparation conditions, such as deposition time, temperature, and annealing temperature. The optical and electrical properties of the ITO thin film and nanorods are discussed and characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), and transmittance analyses.

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The effect of fabrication conditions on the improved photoluminescence of green-emitting $Ca_3Sc_2Si_3O_{12}:Ce^{3+}$ phosphors

문정호, 박병규, *이경남, **도영락

*국민대 화학과 *국민대 생명나노과학부 **국민대 생명나노화학과*

We have studied a novel green-emitting phosphor that is a suitable color conversion material for white light-emitting diodes (LEDs). $Ca_3Sc_2Si_3O_{12}:Ce^{3+}$ phosphor was synthesized by a solid-state reaction. The phosphor was excited by a Xe-lamp and has a 450nm wavelength and emits a green-emitting luminescence wavelength of 507nm. $Ca_3Sc_2Si_3O_{12}:Ce^{3+}$ phosphor was annealed at high temperature for 5 hours under a reducing atmosphere (5% H_2 + 95% N_2). The calcined products were ground and measured. The optimum conditions of $Ca_3Sc_2Si_3O_{12}:Ce^{3+}$ phosphor were evaluated by Ce mol percent (mol%) and annealing time (3~6 hours) at 1350℃. The structural and optical properties of the $Ca_3Sc_2Si_3O_{12}:Ce^{3+}$ phosphor with various activator concentrations and annealing times at 1350℃ were investigated by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Photoluminescence (PL) measurements.

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Tunable color temperature of $Y_3Al_5O_{12}:Ce^{3+}$ white light-emitting diodes using a light-recycling filter for warm white LEDs

오정록, *도영락

*국민대 화학과 *국민대 생명나노화학과*

Recently, we investigated a simple approach for the design of blue excitation light transmitting and phosphor-yellow-emission-light reflecting dielectric multilayers (SiO_2/TiO_2) to recycle the backward emission of $Y_3Al_5O_{12}:Ce^{3+}$ (YAG:Ce) yellow phosphors on top of a blue InGaN light-emitting diode (LED) cup. The enhancement of luminous efficacy and variation of the CCT and color rendering index (CRI, Ra) of LRF-assisted white YAG:Ce LEDs were studied with three reflectance colors (yellow, orange, and red) in LRFs for warm white indoor illumination. The lowest CCT (3720K) was observed with YAG:Ce single-phosphor converted white LEDs from reddish LRF-assisted LEDs with enhanced luminous efficacy (1.58 fold) and a reasonable CRI (Ra > 75).

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Fabrication of a transparent thin film using Y_2O_3: Yb^{3+} Tm^{3+} up-conversion phosphor by the Pechini-type sol-gel method

박병규, *도영락

*국민대 화학과 *국민대 생명나노화학과*

Blue up-conversion luminescence of flux ($LiCO_3$) containing Yb^{3+} and Tm^{3+} co-doped Y_2O_3 thin-film phosphors were grown on a sapphire substrate prepared by the Phchini-type sol-gel process using a spin-coating technique. Yttrium nitrate, ytterbium nitrate, thulium nitrate, and citric acid were used as precursor materials. Y_2O_3: Yb^{3+} Tm^{3+} exhibits strong blue up-conversion luminescence under excitation of a 978nm IR laser. To enhance the optical properties of Y_2O_3: Yb^{3+} Tm^{3+} thin-film phosphors, we studied various preparation conditions, such as annealing temperature and flux concentration. Structural and optical properties were investigated by X-ray Diffraction (XRD), Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), and Photoluminescence (PL).

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Preparation and Characterization of Hollow-type Metal Oxide Particles

강영주, 양재훈, 한양수, *박인

*(주)나노스페이스 나노물질연구소 *한국생산기술연구원 패키징기술지원센터*

Hollow-type SiO_2 particles with the size of 0.5 ~ 2.0 μm are prepared by an inorganic template and seed growth process. At first, size controlled Fe_2O_3 core particles are synthesized by the forced hydrolysis - seed growth reaction of mixed iron salts in the presence of base. The iron oxide surface is then coated with SiO2 using tetraethoxysilicate (TEOS) by typical Bayer process to form core-shell type nanocomposite particles. The core material is then removed by acid washing with hydrochloric acid solution, resulting in the hollow-type SiO_2 spheres. It is found that the cavity size is closely controlled by the size of core particle. The particle characteristics including size, shape, pore size, and pore volume will be discussed on the basis of XRD, SEM, TEM, and nitrogen adsorption-desorption isotherms.

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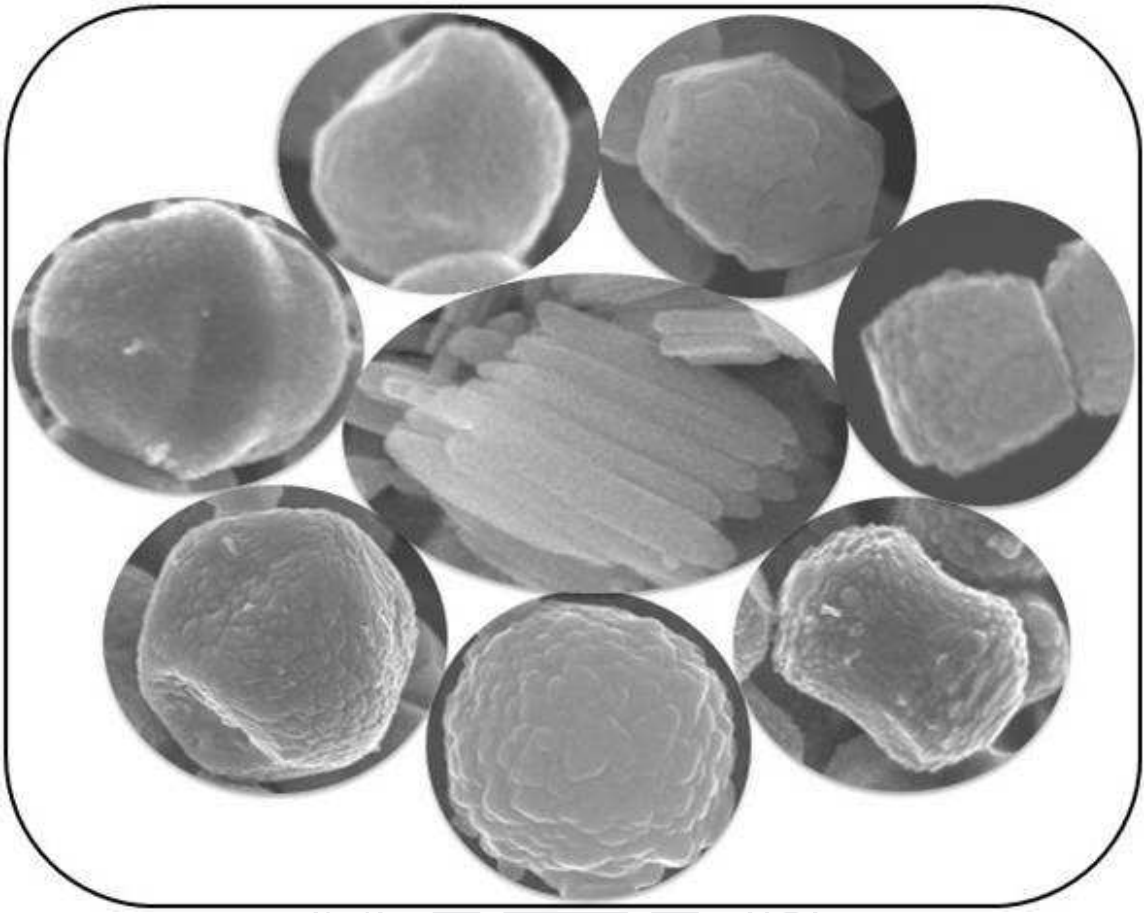
Shape Control Synthesis and Characterization of Hematite α-Fe2O3 Nanostructures

Nitin Chaudhari, *김민식, *김정호, *유종성

*고려대 소재화학과 *고려대 신소재화학과*

Shape and size control will always be an intriguing issue in the nano world. The ability to control the structure of metal oxide materials at a nano and micrometer-length-scale impart new unique characteristic features to the material, subsequently helping in development of new technologies [1, 2]. As various shapes and sizes are 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, chelating or surfactant-active agents, which have to be removed after the reaction. Thus, developing spontaneous generations of novel patterns and tailored structures and shapes by a template-free simple method remains a challenge. We have successfully controlled the shape, size and morphology of hematite α-Fe2O3 without any template or surfactant. Various sized rods and diverse shape control such as hexagonal-prisms, cube, dumbbell-like, bowl-like, hemisphere, sphere, and so on were achieved by one step easy and straightforward synthetic routes [3, 4]. We believe these synthesis methods will give new insight to the development of magnetic nanostructures for the potential applications.References1. Y. Sun and Y. Xia Science, 298, 2176 (2002).2. Y. D. Yin, and A. P. Alivisatos Nature, 437, 664 (2005).3. N. K. Chaudhari and J. S. Yu J. Phys. Chem. C, 112, 19957 (2008).4. N. K. Chaudhari, H. C. Kim, D. R. Son and J. S. Yu Cryst. Eng. Comm., 11, 2264 (2009).



THE KOREAN CHEMICAL SOCIETY

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Phenothiazine-based sensitizers with different conjugated linkers for efficient dye-sensitized solar cells

김세훈, *김재필

*서울대 공과대 재료공학부 *서울대 재료공학부*

We designed and synthesized phenothiazine-based sensitizers with different conjugated linkers for dye-sensitized solar cells (DSSCs). New organic sensitizers had furan (SHW-8), thiophene (SHW-9), and 3,4-ethylenedioxythiophene (SHW-10) moieties as conjugated linkers. The photovoltaic properties was measured in both the absence and presence (10mM, saturated concentration) of chenodeoxycholic acid (CDCA) as co-adsorbent. The performances of device fabricated in the presence of CDCA were higher than those achieved in the absence of CDCA. Among the sensitizers, the highest solar energy-to-electricity conversion efficiency was achieved with SHW-8 which had the maximum η value of 6.58% (Jsc = 12.18mA/cm2, Voc = 771.7mV, FF = 70.02%) improved above 24% compared to the reference 5.29% (PTZ1) under the same conditions (at AM 1.5 illumination).

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Tuning the HOMO Energy levels of Diphenylaminothiophene Dyes for Efficient Dye-sensitized Solar Cells

사공천, 김재필

서울대 재료공학부

가시광선 흡수영역을 확장시키기 위해 전자주개 그룹에 기존의 triphenylamine 보다 donating ability 가 향상된 diphenylaminothiophene 을 도입하였으며, HOMO energy level 이 광전변환효율에 미치는 영향을 분석하기 위해 치환기 (butoxy, benzene, thiophene, EDOT)를 도입하여 HOMO energy level 을 미세하게 조절한 6 종의 신규 염료를 설계 및 합성하였다. 이를 바탕으로 합성된 신규 염료의 분광특성 및 전기화학적 특성을 분석하였으며, 염료감응 태양전지를 제작하여 흡수파장과 HOMO energy level 이 광전변환효율에 미치는 영향에 대해 고찰하였다. 추가적인 전자주개 그룹 (alkoxy)과 bridge group (benzene, thiophene, EDOT)을 도입함에 따라 흡수 영역은 크게 장파장화하여 전색체에 가까운 특성을 나타내었으며, 염료의 HOMO energy level 과 전해질의 redox potential 간의 차이가 0.3eV 이상 positive 해야 DSSCs 의 구동이 원활하게 일어나는 것을 알 수 있었다.

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Preparation of Hollow-type Metal Oxide Particles with Controlled Morphology

강영주, 양재훈, 한양수, *박인

*(주)나노스페이스 나노물질연구소 *한국생산기술연구원 패키징기술지원센터*

Hollow-type metal oxide particles with various cavity morphology are prepared by inorganic template method using Fe_2O_3-SiO_2 core-shell composite particles. The core Fe_2O_3 particles with the shape of spherical, peanut, ellipsoidal, cubic, and hexagonal plate are firstly synthesized. In order to obtained sub- and micron sized core particles seed growth method was used in the forced hydrolysis reaction. Then SiO_2 layer with the thickness of 40 ~ 50nm is deposited on the surface of pre-prepared core particles by the two-step coating process. Subsequently the core material is leached completely by washing with 0.1N-HCl solution at the elevated temperature, leading to the hollow-type SiO_2 particles with preserving the cavity morphologies which are identical to those of core particles. Such prepared hollow type particles were tested as light diffusing agent in the optical coating materials.

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Mesoporous Carbon Nanofibers with uniform open mesopore array on the wall

김민우, *김정호, *김민식, 송민영, 임신묵, **양대수, **Nitin Chaudhari, kiran chaudhari, ***유종성

*고려대 소재화학과 *고려대 신소재화학과 **고려대 신소재화학*

Mesoporous carbons have attracted considerable interest due to their diverse properties such as, high specific surface area, ordered pore channels large pore sizes; finding applications in diverse filed spanning from catalysis, separation, as electrode materials, and gas storage. With the advent of mesoporous carbons, hierarchical mesoporous carbon materials, such as mesoporous carbon nanofibers (MCNF) and mesoporous-macroporous carbon (MMC) have attracted considerable attention due to their interesting structures and properties. Anodic aluminum oxide (AAO) membrane and colloidal crystal are the two typical hard templates used for the preparation of hierarchical mesoporous materials.Herein, we report synthesis of mesoporous carbon nanofibers (MCNF) by using hard template and Ludox TM-40 as silica source, employing replica method concurrently giving rise to open mesopore structure on the wall. 10 wt % of ludox TM-40 was added drop wise to the anodic aluminum oxide (AAO) membrane followed by centrifugation. AAO/silica was dried overnight at 80 °C and the AAO/silica composite formed, was polymerized and carbonized at 700 °C in flowing N2 for 3h. Nanofibers obtained were etched with 48% aqueous HF washed and dried in oven at 80°C. 1M NaOH was used to remove AAO membrane.Removal of the AAO membrane, revealed well interconnected mesopore arrays. Hence successful synthesis of well ordered mesoporous carbon Nanofibers was achieved.

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QSPR models for dielectric constants of polymers based on 2D chemical structure

안민형, 차지영, *김용석, 이성광

*한남대 화학과 *한국화학연구원 화학소재연구단 정보전자폴리머연구센터*

The dielectric constant of polymer is one of the key properties of polymer and affects many electrical applications. In this study, quantitative structure property relationships(QSPRs) were constructed to predict dielectric constant of polymers. The dielectric constant data for polymers was obtained from Bicerano's Book and PoLyInfo database. Chemical structures were parameterized using PreADMET program and 1000 2D descriptors were obtained directly from the structures of repeating units for each polymer, including diverse structural information. The linear and non-linear models are applied on the basis of a various theoretical molecular descriptors selected by the genetic algorithm selection procedure. These results suggest that QSPRs prediction models of dilectric constant permit high throughput experiments of electrical properties from virtual polymer libraries.

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Large area, aligned self-assembly of surface modified single-walled carbon nanotubes

Najeeb.C.K, 창징보, 안대희, 김재호

아주대 분자과학기술학과

Carbon nanotubes (CNTs) are among the most promising materials predicted to impact future nanotechnology owing to their exceptional structural and electronic properties. Aligned organization of nanotubes on a substrate is the primary requirement to exploit their unique electrical, optical and mechanical properties for their realistic potential applications. In our research, we employed surface modification of SWNTs with two different surfactants to meet the specific conditions for the self assembly of single-walled carbon nanotubes (SWNTs) in drop casted or spin coated films. The self assembly of nanomaterials from their surfactant dispersion is based on the shape, aspect ratio, surface charge and lateral capillary force during the drying process. First, we prepared SWNT dispersion with a biosurfactant sodiumdeoxycholate (SDC), which provided a rigid rod-like structure to the CNTs due to the presence of rigid steroid rings. Then, the dispersion was treated with an anionic surfactant, sodium dodecylbenzene sulfonate (SDBS) to generate negative charge on the CNT surface as well as to reduce surface tension of the medium. A large area aligned CNT film was obtained and the degree of alignment was varied with the ratio of SDC to SDBS in the solution.

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Synthesis and Photovoltaic properties of efficient oxazine dyes for DSSCs

이우성, 김재필

서울대 재료공학부

New oxazine dyes with thiophene or furan 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.

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Nitrogen-Doped Hybrid Carbon Nanostructures Induced by Direct Carbonization of Amphiphilic Copolymers for Efficient Electrocatalysis

장유진, 김동하

이화여대 화학나노과학과

Carbonaceous materials have been typically employed as an electrocatalyst support in polymer electrolyte membrane fuel cells (PEMFCs) due to its high electrical conductivity and large surface area when they form a composite with noble metals, e.g., platinum/carbon or palladium/carbon. However, their wide use in commercial applications has been limited by the high cost of noble metals and carbon monoxide (CO) poisoning on the metal surfaces which causes deactivation of metal electrocatalysts, thus resulting in overall decrease in the fuel cell performance. In this respect, it has attracted increasing interest to develop new, effective electroactive materials replacing noble metals and nitrogen-doped (N-doped) carbon is considered as a promising candidate in line with this purpose. In this presentation, we demonstrate a facile, one-step strategy to fabricate N-doped carbon nanostructures with electrocatalytic activity toward oxygen reduction reaction by utilizing amphiphilic block copolymers as a template for the structural control and a carbon source as well.

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Different sized nanoporous TiO2 spheres used as scattering layer in dye-sensitized solar cell (DSSC) for the conversion of photovoltaic energy

유인경, 한송이, **Rawal Sher Bahadur**, 이완인

인하대 화학과

Nanoporous TiO2 spheres of various sizes have synthesized, and the effect of the scattering layer(SL) of nanoporous TiO2 spheres in dye-sensitized solar cell(DSSC) has been studied. Nanoporous TiO2 spheres is prepared by hydrothermal method. For the synthesis of nanoporous TiO2 spheres, the acetonitrile in ethanol, the mixture of H2O and methylamine and the Ti(O-iPr)4 in ethanol were mixed and stirred for 1hr. Highly crystallized nanoporous TiO2 spheres were formed by hydrothermal reaction at 230oC for 5 hr. The size of TiO2 spheres was controlled by hydrolysis reaction between Ti precursor and H2O. The diameter of synthesized TiO2 spheres in pure anatase phase was determined to 250~800nm by TEM and SEM. The main TiO2 layer with a particle size of 10~20nm was formed by doctor-blade method on the FTO glass. And then the SL of nanoporous TiO2 spheres was formed by doctor-blade method. The photovoltaic-conversion efficiency (η) was found to be increased due to the efficient scattering effect of nanoporous TiO2 spheres. Particularly, TiO2 spheres with the size of 450nm was the most efficient scattering efficiency.

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Synthesis of highly crystallized hollow β-MnO_2 for the lithium intercalation/deintercalation process

오규환, 박윤봉

충남대 화학과

Manganese dioxide (MnO_2), which can accommodate significant lithium in the structure, has many polymorphs including α, β, γ and δ forms; among them, it is much more suitable than other forms to use β-MnO_2 with the narrowest [1 × 1] channels as lithium absorbent. Furthermore, β-MnO_2 is not only the most stable in thermodynamics but also very easy to be prepared. Various methods to synthesize β-MnO_2 have been known, such as hydrothermal, sol-gel, chemical precipitation and templating methods, etc. In this work, we have devised the new procedure using the hydrothermal method in order to synthesize a highly crystallized hollow β-MnO_2 which has well-defined morphology and uniform particle size. The physico-chemical properties of the as-prepared material were characterized by thermogravimetric analysis (TGA)/differential thermal analysis (DTA), X-ray powder diffraction (XRD), infrared (IR) spectrometer and scanning electron microscopy (SEM)/transmission electron microscopy (TEM) for the purpose of evaluating the as-synthesized β-MnO_2 as lithium absorbent.

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Study of Gels for Decontaminating Surface by Nonionic Surfactant

방인배, 박윤봉

충남대 화학과

Decontamination gels are capable of both detecting and removing hazardous nuclear and heavy metal contaminants from contaminated surfaces. The gels can be brushed or sprayed onto the contaminated surfaces as solution or dispersion in aqueous media. Upon drying, these coatings that can easily be peeled or stripped from the surface. Gels typically consist of inorganic viscositier, surfactants and decontaminants. Surfactants have been well used because of their effect on the drying time of the gel, cracking, and adhesion to the surface. In this work, we have selected dioxyethylene glycol hexyl ether and polyethylene glycol with different values of HLB. The Hydrophilic-Lipophilic Balance of a surfactant is a measure of the degree to which it is hydrophilic or lipophilic. We will report the properties of the decontamination gels such as drying time, degree of cracking, amount of the dry residue, detachment property, and viscosity.

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Preparation and characterization of M@SiO_2 (M = Ag, Au) core-shell in silica sol

강병규, 김유혁

단국대 첨단과학대학 화학과

Noble metal nanoparticles coated with silica are produced by reducing noble metal compounds with reducing reagents in the presence of NaOH-stabilized, active silicic acid, which is generated by ion-exchange method from water glass. A hydrothermal synthetic method is explored for the synthesis of M@SiO2 core-shell in silica sol with thick silica shell. Control experiments to obtain various shapes and sizes are discussed in terms of metal compounds and reducing agents. The formation of metal nanoparticles and M@SiO_2 core-shell is confirmed by UV-visible absorption spectra, transmission electron microscopy (TEM) and energy dispersive spectroscopy (EDS) data.

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A Fusion of SPR and FRET Sensing System for Highly Accurate and Selective Immuno-sensing

이재욱, *홍성철, Sun Fangfang, **zhou hongjian, **Syed Rahin Ahmed, *이재범

*부산대 나노융합기술학과 *부산대 나노메디컬공학과 **부산대 나노융합기술대학*

Immuno-sensing for high accurate and selective sensing was performed by fluorescence spectroscopy and surface plasmon resonance (SPR), respectively. Combined structure of two fluorescent CdTe Nanoparticles (CdTd NPs) with bovine serum albumin (BSA) and anti-BSA was fabricated in PBS buffer for fluorescence analysis of fluorescence resonance energy transfer (FRET). Furthermore, the same bio-moieties were immobilized on Au plates for SPR analysis. Naturally- driven binding affinity of immuno-moieties induced FRET and plasmon resonance angle shift in the nanoscale sensing system. Interestingly, the detection limits were uniquely different in two systems: e.g., SPR spectroscopy was suitable for highly accurate analysis to measure in the range of $10^{-15\sim-10}$ ng/mL while the CdTd NPs fluorescent sensing system was relatively lower sensing ranges in $10^{-10\sim-6}$ ng/mL. However, the CdTd NPs sensing system was larger than the SPR sensing system in terms of sensing capacity per one specimen. It is, therefore, suggested that a mutual assistance of FRET and SPR combined sensing system would be a potentially promising candidate for high accuracy and reliable in situ sensing system of immune-related diseases.

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Magnetic molecularly imprinted nanoparticles for recognition of lysozyme

surong mei

창원대

Molecular imprinting is an attractive technique for preparing mimics of natural, biological receptors. Nevertheless, the imprinting of macromolecule remains a challenge due to their bulkiness and sensitivity to denaturation. In this work, we presented a method for preparing multifunctional lysozyme imprinted nanoparticles (magnetic susceptibility, molecular recognition and environmental response). The magnetic susceptibility was imparted through the successful encapsulation of Fe3O4 nanoparticles. The selective recognition for lysozyme depended on the molecularly imprinted film. Moreover, it was also the hydrophilic stimuli-responsive polymer, which could undergo a reversible change of imprinted cavity in response to a small change in the enviromental conditions. Thus, magnetic molecularly imprinted nanoparticles had high adsorption capacity (0.11 mg mg-1), controlled selectivity and direct magnetic separation (22.1 emu g-1) in crude samples. Finally, a sensitive method was developed for determination of lysozyme in human serum samples using MIPs nanoparticles for preconcentration and purification of lysozyme and chemiluminescence as the detection method. The results indicated that the spiked recoveries were changed from 92.5 to 113.7%, and the RSD was lower than 11.8 %.

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라포나이트에 층간삽입된 철화합물의 합성연구

양승규, 김유혁

단국대 첨단과학대학 화학과

라포나이트는 층 구조를 이루는 syntheictic clay 로 층사이에 Na+ 이온을 유기 및 무기 양이온으로 교환하여 이들 이온이 함유된 라포나이트를 합성할 수 있다. 본 연구에서는 이온 교환법을 이용하여 라포나이트에 철이온이 함유된 라포나이트를 합성 후 2,2'-bipyridyl, 1,10- phenanthroline 등의 리간드와 반응하여 이들 리간드를 갖는 철화합물의 라포나이트 층간삽입 화합물을 합성하였다. 또한 라포나이트에 Ferric ammonium sulfate 와 NaBH4 를 이용한 화학적 환원 후 공기중에 약 3 일간 산화시켜 얻어진 화합물에 위의 리간드를 반응 후 얻어진 층간 삽입화합물을 비교 연구하였다. 산화된 철 화합물의 확인을 위하여 이들 졸을 동결 건조 시킨 뒤 미분을 만들어 IR 및 XRD 로 확인하였다.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Probing optical properties of noble metal-ZnO nanorod heterostructures

박영석, 최지혜, 채희권

서울대 화학교육과

Noble metal-semiconductor heterostructures have been intensively pursued for their potential applications involved with solar energy harvesting and photocatalysis. In particular, the efficiency of photocatalytic activity has been improved by achieving novel heterostructures between plasmonic nanoparticles and semiconducting nanostructures. One-dimensional ZnO nanocrystals with large band gaps, which can be tuned by changing the confined size and shape, are knows as biocompatible materials with photocatalytic activity and characteristic photoluminescence, and their heterostructures with metallic nanoparticles have exhibit superior efficiency of catalytic activity. Herein, we propose a wet chemical route for preparing the heterostructures between ZnO nanorods and noble metal nanoparticles such as Ag and Au. By overcoming site-specific deposition of metallic nanoparticles on the surface of ZnO nanorods, heterostructures surrounded by well-distributed metallic particles could be prepared, and the optical properties and photocatalytic activity of the heterostructures were investigated.

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Facile Process to Synthesize Mesoporous Silica Nanoparticles (MSNPs)

김원희, *이혜선, **장정호, 박상언

*인하대 화학과 *연세대 신소재공학과 **한국세라믹기술원 바이오IT융합센터*

We synthesized highly ordered mesoporous silica nanoparticles (MSNPs) via facile synthesis process. The self-assembly of silica species and surfactant P123 and the formation of mesoporous silica nanoparticles occur following the hydrolysis and condensation of silica precursor TEOS in solution. We reported the effect of copper(Ⅱ) ion for control particle size. The MSNPs were prepared by copper(Ⅱ) ion addition in micellar solution. The particle size has been easily controlled by different molar ratio of surfactant / copper(Ⅱ) ion. MSNPs were characterized by SEM, DLS, XRD, and BET isotherm analysis. As a results, BET isotherms of materials were retained, but particle size was changed from 2~3μm to 500~600 nm. This synthesis is provided to synthesis process easier and can be used for many applications

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Evaluation of Novel Gd (III) Labeled MRI Contrast Agents

kiran kumar

창원대

Magnetic resonance imaging (MRI) is a non-invasive imaging technique, extensively used in the clinic, which allows for high resolution pictures of a whole-organism to be obtained over extended periods of time. The technique is often enhanced by the use of contrast agents (CAs). Among them, paramagnetic gadolinium chelates hold a prominent position. In general, these agents are injected systemically and serve to passively and nonspecifically enhance the signal by increasing the longitudinal relaxation rate (1/T1) of surrounding water molecules. However free Gd(III) causes to Nephrogenic Systemic Fibrosis (NSF). In this context, it should be noted that the complex stability, solubility and contrast ability are challenges in development of novel conjugates. In the frame of a research program aiming at the development novel MRI contrast agents, we have designed glucuronamide, diethylenetriaminepentacetic acid (DTPA) complexes with Gd(III).

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Gas Sensing Properties ZnO Nanoflowers Decorated with Au Nanoparticles

Saji Thomas, *정운룡, 김동하

*이화여대 화학나노과학과 *연세대 신소재공학과*

As an n-type II-IV semiconductor with large exciton energy (60MeV) and wide band gap (3.37 eV at room temperature), zinc oxide (ZnO) has found potential applications in photonics, light emitting diodes, field effect transistors etc. Distinctive properties like high mobility of electrons and good thermal, chemical stability under operating conditions make ZnO a prominent element among various gas sensors. The sensing performance can be further improved by adding small amount of metals or metal oxides. The metal dopant acts as a catalyst to improve the surface reactions of ZnO towards gas sensing. Here, we report synthesis and characterization of flower like ZnO nanostructure through a simple catalyst and template free hydrothermal route followed by decoration with citrate capped gold (Au) nanoparticles (NPs), where zinc acetate was used as ZnO precursor and NaOH as oxidizing agent. The morphology was explored using SEM. XRD and TEM were used to study the crystalline structure of ZnO nanoflowers. ZnO nanorods connected each other through contact via one end, like a flower fashion, renders electrons to travel from one rod to another by tunneling. Gas sensors based on pure and Au NPs decorated ZnO nanoflowers were then fabricated. The sensing property of the obtained nanostructures was investigated using ethanol gas as analyte.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Work function modulation of schottky barrier using different terminal group of thiolated molecule in carbon nanotube sensor

안대희, Najeeb.C.K, 강원석, 김재호

아주대 분자과학기술학과

Single walled carbon nanotube (SWNT) have been studied due to potential applications in various fields, such as field-effect transistor, flexible electrode, chemical sensors and probe tips. Especially, electrode biosensor has shown great promise in label-free detection, higher sensitivity and miniaturized device.In this study, we fabricate carbon nanotube sensor based on Schottky barrier effect of metal-semiconductor (carbon nanotube) junction. Carbon nanotube behave like a p-type semiconducting thin film in this device and their sensitivity depends on the Schottky barrier at the metal-nanotube contacts. We designed metal-nanotube contact area as a sensing surface. The sensing mechanism of this carbon nanotube sensor mainly used the conductance drop by the charge gating effect which is derived from the immobilization of molecules or the interaction between probe and target molecules onto the sensing surface. we try to modulate work function at metal-nanotube junction, using four thiolated molecule with different terminal group. Conductance drop reflect the work function modulation according to the different of terminal group. this results indicate that carbon nanotube sensor based on schottky barrier effect can apply to the detection of charged molecule such as protein or DNA.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Artificial Eumelanin Nanoparticles with Excellent Dispersibility and Free Radical Scavenging Property

주국연, 이진규

서울대 화학부

A novel synthetic method was developed to prepare size-controllable eumelanin nanoparticles with excellent water dispersibility; eumelanins are well known bio-polymers that are widely distributed in many parts of living organisms exhibiting many interesting properties and various biological functions. Eumelanin nanoparticles were synthesized with size control through neutralization of dopamine hydrochloride with NaOH followed by spontaneous air oxidation of dopamine. Although the particle characteristic of natural melanins was understood to be significantly affected by the biological and structural environment, eumelanin nanoparticles can be realized through the chemical reactions only. Furthermore, eumelanin nanoparticles are smaller than 100 nm showed excellent dispersion stability in water and surface modified eumelanin nanoparticles could be stable in biological medium such as buffer solution and serum as well, which is essential for use in many related biological investigations. Details on synthesis and characterization of artificial eumelanins and their interesting feature of radical scavenging activity will be discussed.

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Characterization of properties as Molten Salt Electrolytes based on mixtures of alkali-metal halides in the Thermal Battery

김병기, 박윤봉

충남대 화학과

Molten salt thermal batteries are activated by raising their temperature above the melting point of the salts 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. For the long-life thermal battery, it is important to have the electrolyte with not only the low melting point but also the high ionic conductivity. In order to evaluate the ionic conductivity of electrolytes, we newly designed a U-shaped cell. The validity of the measurements are confirmed by comparing the values of LiCl-KCl, LiF-LiCl-LiBr, LiF-LiBr-KBr and LiCl-LiBr-KBr systems with those reported values in the literature. The ionic conductivities are measured and evaluated from the melting points of the electrolytes to 480℃. These data provide valuable information on the lifetime of the thermal battery as well as the performance of the thermal batteries. The physicochemical properties of electrolytes were also studied by thermogravimetric analysis (TGA)/ differential thermal analysis (DTA), X-ray powder diffraction (XRD) and elemental analysis.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation and Properties of Alginate-Gelatin-Methyl Cellulose /Silver Nano Particles based Antimicrobial Food Packaging Films

서민호

창원대 화학과

Food quality and safety are major concerns in the food industry. Antimicrobial packaging can be considered an emerging technology that could have a significant impact on life and food safety. Antimicrobial agents in food packaging can control the microbial population and target specific microorganisms to provide greater safety and higher quality products. In this work, we designed and prepared Alginate-Gelatin-Methylcellulose based films. Silver nanoparticles (AgNPs) were loaded into the film, followed by AgNPs added to the polymer solution before casting. The presence of silver nanoparticles was confirmed with scanning electron microscopy, X-ray diffraction, Fourier transform infrared spectroscopy. Mechanical properties of the films like Tensile strength and percentage elongation at break were measured. The silver-nanoparticle-loaded films were investigated for its antimicrobial properties against Escherichia coli.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of cephalexin Loaded Poly(N'-Isopropylacrylamide-co-N-Acryloyl-L-alanine) Hydrogels and Its In Vitro Release Studies

김용현

창원대 화학과

Thermosensitive hydrogels composed with N'-isopropylacrylamide (NIPAm) and N-Acryloyl-L-alanine (ALA) and crosslinked by N,N-methylene bisacrylamide (MBA) were prepared using free radical polymerization. Cephalexin (CPX) was loaded in to copolymeric hydrogels successfully by swelling equilibrium method. Various formulations were prepared by varying the amount of NIPAm, ALA, and MBA. The CPX loaded gels were characterized by X-ray diffraction (XRD) 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 50 to 70 % measured using UV-vis method at 262 nm. The swelling studies were indicated a dependence of extent of monomer and crosslinker ratio in the hydrogels.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Optical Property of Heptamethine cyanine derivatives on Near-Infrared

조보배, 심현오, 송재미, 김영순

동국대 화학과

Many of cyanine dyes used on industry as photoinitiator, illuminator and absorbent. It have good thermal stability, solubility and high molar absorbtion efficiency as using in upper field. We have a interest in the optical properties of the heptamethine cyanine dye, absorb the near infrared, that have useful character as photoinitiator. However their photostability is weak by ultra violet, it influence to sustainability of energy transfer. In this study, we changed the structure of side and bridge form to enhance the photostability. we synthesized cyanine derivative and comparison with each structure such as substitution of side, shape and number ring on bridge. As a result, we realized the tendency of photostability on sturcture of hetpamethine cyanine dyes.

일시: 2010년 10월 14~15일(목~금) 2일간

장소: 대구엑스코

발표코드: **MAT.P-109**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

Novel synthetic route for coronene chromophores and their applications

최준, 김재필

서울대 재료공학부

A new synthetic route of core extended perylene chromophores was suggested. New types of coronene derivatives that have sterically demanding phenyl substituents at their bay positions could be synthesized by means of a simple one-step reaction with this route. The absorbance of synthesized coronene derivatives were hypsochromically shifted compared with that of the perylene derivatives, leading to very stable yellow chromophores with high molar extinction coefficients which are generally difficult to obtain. Therefore, they could be successfully used as yellow color compensating dyes of LCD color filters. In addition, they had bright fluorescence with a high quantum yield which suggests various demanding applications.

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장소: 대구엑스코

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis of bay-substituted perylene diimide dyes with low permittivity for black matrix

육심범

서울대 재료공학부

One of the major issues in display technology is thickness of panel. Using dyes instead of carbon black, thinner black matrix can be made. In this study perylene dyes have been designed and synthesized. To enhance thermal and light stability, aryl substituents were linked with C-N coupling. The optical and thermal properties of dyes were measured with UV-spectrometer, TGA and DSC.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Direct transformation of the exfoliated two dimensional MnO_2 nanosheets to one- dimensional Mn_3O_4 Nanorods

이나라, 이지연, 정현

동국대 화학과

A novel synthetic route has been developed to prepare manganese oxide nanorods. Using unilamellar manganese oxide nanosheets as starting materials, we succeeded in obtaining manganese oxide nanorods. The starting materials, exfoliated manganese oxide nanosheets, were obtained by intercalation and delamination reaction of the layered manganese oxide with tetrabutylammonium cation. The transformation of layered MnO_2 nanosheets to Mn_3O_4 nanorods was successfully achieved by simple calcination process. Physicochemical characterization and transformation mechanism study were performed by using X-ray diffraction (XRD), High-resolution transmission electron microscopy (HR-TEM) and Field-emission scanning electron microscopy (FE-SEM). The component and thermal behavior of the sample were respectively measured by Fourier transform infrared (FT-IR) spectroscopy and thermal analyses, including thermogravimetry (TG) and differential thermal analysis (DTA).

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Synthesis and Characterization of the SiO_2 coated Cobalt monoxide Nanoshells Structure with Controlled Shape and Size

권민재, 최민아, 정현

동국대 화학과

CoO(core)/SiO_2(shell) nanoparticles and nanorods were prepared by reverse microemulsion method. To fabricate core materials, the shape controlled cobalt oxide nanoparticles were obtained by thermal decomposition method of Co-(oleate)$_2$. The cobalt precursor was synthesized by simple complex reaction of cobalt chloride hexahydrate and sodium oleate molecules. The shape and size of the cobalt oxide nanoparticles were easily controlled by changing the reaction conditions, such as the heating ratio (0.5, 1.0, 2.0, 3.0 and 4.0 ℃/min) and the crystal growth time (30, 60 and 120 min) during thermal decomposition reaction. When the heating ratio was increased, the aspect ratio of the CoO nanorods was gradually decreased until the formation of pyramidal shaped CoO nanocrystals. SiO_2 coating on core cobalt oxide nanoparticles was performed by hydrolysis and condensation reaction of tetraethyl orthosilicate (TEOS) in the water phase of reverse microemulsion system. The physicochemical characterizations of the obtained CoO(core)/SiO_2(shell) nanoshell materials were performed by X-ray diffraction (XRD), high-resolution Transmission electron microscopy (TEM), Scanning Electron Microscope (SEM), Inductively coupled plasma (ICP) and Fourier transform infrared (FT-IR).

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Characterization of Nickel Hydroxide Nanoparticlesby using ɣ-ray Radiation

심은하, 최정화, 정현

동국대 화학과

A novel synthetic route has been developed to prepare nickel hydroxide with intercalated nitrate anions. It was successfully synthesized by using ɣ-ray irradiation at room temperature under atmospheric condition without any stabilizer or base molecules. Under ɣ-ray irradiation, it leads to the formation of layered nickel hydroxylnitrate compounds and the generation of hydroxyl anion by way of radiolysis reaction of hydrated nickel nitrate in 2-propanol. Structural and morphological characterizations were performed by using power X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), and high resolution transmission electron microscopy (HR-TEM). The component and thermal stability of the product were respectively measured by Fourier transform infrared (FT-IR) spectroscopy, elemental analysis, and thermal analyses, including thermogravimetry (TG) and differential thermal analysis (DTA).

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발표종류: 포스터, 발표일시: 금 15:00~17:00

The fabrication of nanoporous TiO_2/SnO_2 with half hollow sphere structure and its performance as electrode for dye sensitized solar cell

박유림, 류광선

울산대 화학과

The SiO_2 nanoparticles were synthesized as core material. TiO_2 nanoparticles were obtained the hydrolysis reaction of titanium isopropoxide sol-gel method for formation on the surface of SiO_2. In addition, the 1, 5 and 10 wt% $SnCl_2.2H_2O$ were added in this sol-gel solution for making the SnO_2 nanoparticles. For making TiO_2/SnO_2 nanoparticles with half hollow sphere structure, we removed SiO_2 using NaOH solution. The crystal phase, crystal shape, and surface properties of the metal oxide nanocrystals were studied by X-ray diffraction, scanning electron microscopy, transmitting electron microscopy, and Brunauer-Emmet-Teller measurements. The photovoltaic performance of the TiO_2/SnO_2 nanoparticles with half hollow sphere structure was measured. The new kind of porous TiO2 solar cell exhibits an overall conversion efficiency of 7.36% at 100mW/cm^2. The short circuit photocurrent (Isc) and open circuit photovoltage (Voc) were increased and the conversion efficiency was improved.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Controlling Intermetallic Bonds by Guest Alkali Metals in The Mixed-metal Host Framework, $Nb_xTa_{1-x}PS_6$

이은실, *윤호섭

*아주대 에너지시스템학부 *아주대 화학과*

The new mixed-metal thiophosphates, $K_y(Nb_xTa_{1-x})PS_6$(A = K, Rb; M = Nb, Ta) have been synthesized by using reactive alkali metal halide fluxes and structurally characterized by single-crystal X-ray diffraction techniques. The title compounds are closely related with $TaPS_6$ and their structures are isostructural with the previously reported quaternary alkali metal thiophosphates, A_yTaPS_6 (A = K, Rb). The structure of the title compounds contains 3-dimensional open framework anions, $[MPS_6^{y-}]$ (M = Nb, Ta) with the empty channel which disordered alkali metal cations, K^+ and Rb^+ are located in. The most interesting feature of the structures is the interatomic M-M distances in the dimeric$[M_2S_{12}]$ units. The M-M distances are varied, 3.195(1)Å for $K_{0.41}(Nb_{0.66}Ta_{0.34})PS_6$, 3.233(1)Å for $K_{0.36}(Nb_{0.50}Ta_{0.50})PS_6$ and 3.200(1)Å for $Rb_{0.38}(Nb_{0.23}Ta_{0.77})PS_6$. These distances are significantly shorter compared to that in $TaPS_6$ (3.361(1)Å). Substantial decrease of M-M interatomic distances by the insertion of alkali metals implies that the electrons released by alkali metals are transferred to the d-orbitals of the metals. As a result, the intermetallic bond begins to form and the bond strength can be controlled gradually by the amount of the alkali metals.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

A fast pH-responsive hydrogel: synthesis and application

윤성학

창원대 화학과

In the past few years, there has been increased interest in the development and applications of hydrogel, specifically as a new class of biomaterials. In some cases, the hydrogels can absorb specific stimuli and pH. Hydrogels are cross-linked polymer networks swollen in water. Smart hydrogels undergo a swelling-deswelling transition in response to certain stimuli such as a change in pH. We propose a hydrogle of new design, Confirm a character of the hydrogel.

THE KOREAN CHEMICAL SOCIETY

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The mechanistic study of the metal-chalcogenide nanopartcles

정연구, 이진규

서울대 화학부

The thermal decomposition of Cd(OA)2, metal precursor, and synthesis of CdSe nanoparticles by hot-injection method was studied in order to understand the formation of the metal chalcogenide nanoparticles. The analysis results showed that the initial decomposition of metal precursor was similar to thermal decomposition pathway of single molecule precursor. The nucleophilic attack of amine to the most electron-deficient carbonyl carbon of the lignads at high temperature is supposed to initiate the decomposition to generate Cd(OH)2 or CdO moiety. The metal-chalcogenide nanoparticles were formed from reaction of intermediate and chalcogenide source. We have confirmed the isolated intermediates and side products by TEM, FAB-MS, XRD etc.

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Preparation of lithium contaning oxynitrides with layered perovskite structure

이은혜, 김영일, *김성철, *김승주

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Lithium containing oxynitrides $LiLaTa_2O_{7-3x}N_{2x}$ have been prepared by ammonolysis of Dion-Jacobson type layered perovskite $LiLaTa_2O_7$ at 550-700℃. Upon the ammonia treatment, the initial white oxide powder turned beige to light pink, depending on the heating temperature. Powder X-ray diffraction analysis showed that the partial nitridation lead to the increase of *a* and decrease of *c* parameters. For both the sample color and lattice parameters, the larger changes were observed from the higher ammonolysis temperature. Using the UV-visible absorption spectroscopy, the band gap of pristine oxide and oxynitride samples were measured as 4.1 and 2.8-2.1 eV, respectively. As revealed by the thermogravimetric analyses in air and N_2, the oxynitride derivatives have an improved thermal stability.

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Synthesis and Characterizations of Orthorhombic $Li_{2.35}(V_{1.74}Nb_{0.26})(PO_4)_3$

류재민, *윤호섭

*아주대 에너지시스템학부 *아주대 화학과*

The title compound was prepared and structurally characterized by single-crystal X-ray diffraction techniques. This compound could be a promising material as a cathode for lithium-ion batteries. It possesses both good ion mobility and high lithium capacity because of its ability to extract all lithium ions from the lattice reversibly. This compound crystallizes in the space group Pbna of the orthorhombic system with four formula units in a cell dimensions, a=8.622(0) Å, b=8.672(0) Å, c=12.083(0) Å V=903.6(1) $Å^3$. The structure of the compound is comprised of (V/Nb)-centered octahedra and P-centered tetrahedra. These polyhedra are sharing O atoms to form a three-dimensional framework with huge empty space. Li^+ ions reside in this space to stabilize the structure through electrostatic interaction. In this presentation, the optical characteristics as well as the electrochemical properties of the title compound will be discussed.

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A Study on the Decomposition Process of $Gd_2(OH)_5NO_3 \cdot xH_2O$ and its Keggin-ion Pillared Complexes

이승수, *윤호섭, *강준건

*나노정보융합기술연구소/아주대 *아주대 화학과*

Thermal decompositions of gadolinium hydroxynitrate($Gd_2(OH)_5(NO_3) \cdot xH_2O$, GHN) and its Keggin-ion pillared complexes, $Gd_2(OH)_5(Z^{n-})_{1/n} \cdot yH_2O$($Z^{n-}$= $PMo_{12}O_{40}^{3-}$ and $SiMo_{12}O_{40}^{4-}$, hereafter denoted as Gd-PMo_{12} and Gd-$SiMo_{12}$) have been studied using TG-DSC-QMS, FT-IR and XRD techniques. TG-DSC-QMS data show the three- step mass losses are observed in GHN: dehydration(RT~200 ℃), dehydroxylation (200~350℃) and transformation into Gd_2O_3 with losing NO, NO_2, H_2O and O_2(350~600℃). In case of Gd-PMo_{12} and Gd-$SiMo_{12}$, dehydration precess is shrinked noticeably compared to GHN and gradually increases upon the temperature, which means water molecules dominantly exist as the constitutional ones. Dehydroxylation occur between 200 and 380 ℃ with the evolution of H_2O and CO_2. In contrast to the host material, the Keggin-ion pillared complexes did not show no weight change in the wide temperature range(380~800℃) except a sharp exthothermic peak due to the phase transition of Keggin unit on DSC thermogram. The pillared samples still represent well-defined XRD patterns upto 400℃ for Gd-PMo_{12} and up to 500℃ for Gd-$PSiMo_{12}$, which supports the Keggin uint between the GHN slabs could be maintained up to the high temperature region.

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Highly efficient protein separation with functionalized magnetic nanoparticles

이선영, *안치영, **장정호, 박상언

*인하대 화학과 *고려대 신소재공학과 **한국세라믹기술원 바이오IT융합센터*

This work reported the development of the highly efficient protein separation process with surface functionalization of silica coated magnetic nanoparticles. Magnetic nanoparticles were prepared by coprecipitation of Fe2+ and Fe3+, and then, tetraethyl orthosilicate(TEOS) was directly coated by sol-gel process. The surface modification was performed with functionalized organosilans such as amine-, thiol-, disulfide-, and dodecyl- groups. The silica coating and surface modification are both biocompatible and possessing active groups which can be conjugated to biomolecules such as proteins and enzymes. The protein separation with functionalized magnetic nanoparticles was achieved for model protein such as bovine serum albumin(BSA) and lysozyme(LSZ) at different pH conditions. The work on using silica coated magnetic nanoparticles for protein separation have the advantages such as easy preparation, easy handling, high stability and extensive potential of biotechnology applications.

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Control of anisotropic growth and metal ion doping of ZnO nanorods during growth stage

박영석, 최지혜, 채희권

서울대 화학교육과

One-dimensional anisotropic ZnO nanocrystals have been of particular interest for their potential applications including gas and chemical sensing, UV detectors, and catalysis. Various wet chemical methods have been available for the preparation of ZnO nanorods and wires with different aspect ratios. Control of shape and size of ZnO nanocrystals give rise to the variation of their optical and electrical performance. Although ZnO nanorods and nanowires have been simply synthesized through solvothermal routes, ZnO nanorods with monodisperse diameters were not found from the results of previous mothods. Herein, we describe a seed-mediated solvothermal method to yield thin ZnO nanorods with controlled aspect ratios from 5 to 30 and monodisperse diameters by using organic bases. In addition, doping of metal ions into ZnO nanocrystals during growth stages was performed and investigated.

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Layered Double Hydroxides (LDHs) – Methotrexate Nanohybrid for Chemotherapy

오연지, 최진호

이화여대 화학.나노과학과

In recent years, there has been a great deal of interest in various inorganic nanoparticles because of their potential use as drug or delivery vector. Among them, layered double hydroxide (LDH) has attracted a special attention due to its anionic reservoir capacity, low toxicity and enhanced cellular uptake of loaded drug. In addition, LDHs enable drugs to be delivered effectively to the target site, and eventually increase the therapeutic efficacy with minimum side effects through controlled release manner.In this study, an anticancer drug, methotrexate (MTX), was intercalated into LDHs through co-precipitation route to produce MTX-LDH nanohybrid. According to the Powder X-ray diffraction, spectroscopy analysis and thermogravimetric analysis, MTX molecules were found to be stabilized in the interlayer space of LDHs by electrostatic interaction, without any structural and chemical deformations. From the SEM studies, we found that the MTX-LDH nanohybrid particles were evenly distributed with an average primary particle size of about ~100nm. We also investigated the anti-tumor effect of MTX-LDH nanohybrid in orthotopic breast cancer model, and found that the drug efficacy of MTX-LDH was significantly increased compared to that of MTX only.

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Quantification and bio-application of amine-functionalized silica nanoparticles

정학성, 이진규

서울대 화학부

(3-trimethoxysilylpropyl)diethylenetriamine (DETAS) was employed as a surface ligand for the modification of SiO2 nanoparticles, which has multiple amino groups with two secondary and one primary sites, thereby producing a higher number of amine functional groups. The DETAS-modified silica nanoparticles, SiO2-DETAS, were very stable in alcoholic solution and reasonably stable in acidic (pH < 6) aqueous solution without producing insoluble precipitates. The amount of amino functional groups on SiO2-DETAS was quantitatively analyzed by acid-base titration method, and the effective amount of amino functional groups for the next chemical reaction was determined by treating with fluorescent Rhodamine B isothiocyanate (RITC) molecule. The amino surface groups of SiO2-DETAS could also be easily converted to aldehyde groups by treating with excess amount of glutaldehyde (GA), as one of the well-known bioconjugation protocols, and followed to react with biomaterials having amine functional groups such as antibodies. Quantitative analysis results and interesting application based on those bioconjugation reactions from the multiple amino groups on the surface of SiO2-DETAS will be discussed.

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NiO incorporated Magnetic Mesoporous Silicas for Enhanced Protein Purification Separation System

이지호, *장정호, 박상언

*인하대 화학과 *요업기술원 바이오IT융합센터*

Here we present a method for supported biomaterials in which mesoporous silicas were functionalized with Fe and NiO in a stepwise manner and then used as a host material for adsorption of specific proteins, His-tagged proteins. Mesoprous silicas were combined with iron(II) chloride tetrahydrate for initiating magnetizing process, followed by reduction in H2 media. The nickel(II) chloride hexahydrate was introduced into pore and surface of magnetic mesoporous silicasres (FeMS) by wet impregnation process. The resulting materials were reduced in a flowing of H2 at 500 oC for 2h, thereby producing Ni particles on the surface of the FeMS. The Ni particles were oxidized by exposing them to the air under ambient conditions for two days. The FeMS-NiO was characterized by various state-of-the-art techniques, such as SAXS, WAXS, FE-SEM, TEM, FT-IR, SQUID and nitrogen sorption. FeMS-NiO showed high adsorption level of His-tagged protein from E.coli lysate. In addition, the purified His6-CatA was observed high enzyme activity. It suggests that FeMS-NiO system provides contribution for maintain stable protein structure as well as simplified protein purification process.

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Ketoprofen-LDH Nanohybrid for the Transdermal Drug Delivery System

김학, *최진호

*이화여대 바이오융합과학과 *이화여대 화학.나노과학과*

Layered double hydroxides (LDHs), an inorganic framework, are biocompatible materials which can be used as a drug-delivery system. Ketoprofen is a non-steroidal anti-inflammatory drug for the treatment of inflammation and pain caused by rheumatoid arthritis. In this study, we have successfully synthesized the Ketoprofen-LDH Nanohybrids via co-precipitation method. According to the X-ray diffraction patterns and FT-IR spectroscopy, ketoprofen molecules are well intercalated into the interlayer space of Zn-Al LDH. TG-DTA profiles and HPLC analysis provide the ketoprofen contents arranging in the LDHs. Preliminary ketoprofen release experiments are in progress to examine the release behavior of Ketoprofen-LDH Nanohybrids with controlling the pH and coating solution.

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Electron beam induced structural modifications of Carbon nanotubes

이미진, *신관우, **최재학

*서강대 화학과 *서강대 화학과 및 바이오융합과정 **한국원자력연구소 방사선공업환경연구부*

Irradiation effects of highly energetic electron beams on carbon nanotubes are currently being investigated, as a substitute method of conventional acid treatments with a virtue of economical and environmental issues. Previously, we found that the surface oxidation of CNTs could be effectively achieved. When CNTs were irradiated much longer (~ up to 18,000 kGy), various morphological changes, including scission, wall-thinning, and degradation, were found. In some cases, longitudinal unzipping phenomena, yielding carbon nanoribbons, were also observed. Detailed carbon structures and process conditions will be presented.

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Synthesis and characterization of superparamagnetic Fe_3O_4 nanoaprticles with various sizes and functionalities

최경훈, *정종형, 김용록, *정진승

*연세대 화학과 *강릉대 화학과*

Superparamagnetic nanoparticles have receieved increasing attention interest because of their great potential applications in magnetic fluids, catalysis, biotechnology/biomedicine, manetic resonance imaging (MRI), magnetic recording devices, and environmental remediation. In the present study, we have successfully synthesized of superparamagnetic Fe_3O_4 nanoparitcles with various sizes and functionalities by using a one-step hydrothermal method. The size of Fe_3O_4 nanoparticles can be easily controlled by changing the amount of sodium acrylate and sodium acetate. Also the functionality of Fe_3O_4 nanoparticles provided by the SiO_2 coatings Microstructure and magnetic properties of the Fe_3O_4 nanoparticles are investigated by transmission electron microscopy, vibrating sample magnetometry. The result of this study presents the syntheis of functional magnetic nanoparticles with tunable sizes and various functionalities.

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Enhanced Lithium Storage Capacity and Cycling Performance of SnO2-Layered Titanate Nanohybrid

강주희, *백승민, 최진호

*이화여대 화학.나노과학과 *경북대 화학과*

Porous structure of titanate nanosheets with tin oxide nanoparticles has been realized by exfoliation and reassembling route. No (0l0) peaks corresponding to the layered titanate appear in the powder X-ray diffraction patterns of the reassembled hybrids, suggesting that the titanate nanosheets are randomly distributed between SnO2 nanoparticles to form a highly porous structure. Nitrogen adsorption-desorption measurements clearly show that the hybrid material is fairly high in specific surface area and in mesoporosity (SLangmuir = 346 m2 g-1). The application potential of the present hybrid as an anode material in a rechargeable lithium battery is also demonstrated by electrochemical experiments, where a large reversible capacity with good capacity retention is observed.

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Solubilization of the Antioxidant Resveratrol by Complexation with Cyclodextrin

Laarnie Dumolva, *K. E. Geckeler

*광주과학기술원 나노바이오재료전자공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*

Different antioxidants have been studied for a variety of reasons. In this study, the solubility of the antioxidant resveratrol was enhanced by encapsulating it with cyclodextrin in the solid state. The prescreening of the encapsulated antioxidant was conducted with different ratios and different solvents using UV-visible spectroscopy. We report here the enhanced solubility of the complex formed in water. In addition, other analogues have been investigated, These compounds have been also characterized using different analytical techniques. Finally, the antioxidant activity of these novel compounds will be assessed..

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Fabrication of Hybrid Films Using Diethylzinc and Trihydroxybenzene

한규석, 성명모

한양대 화학과

We fabricated organic-inorganic hybrid polymer films from diethylzinc and benzenetriol using molecular layer deposition under the substrate temperature of 80-230 °C. Infrared and ultraviolet spectroscopic analyses confirm the existence of benzene ring in the hybrid films. The compositional analysis is done by X-ray photoelectron spectroscopy and confirm atomic bonding of organic materials. Spectroscopic ellipsometry indicate the films grow linearly with reaction cycles and also confirm the self-limiting nature of surface reactions at each cycle. Transmission electron microscopy shows that the hybrid films grow uniformly. The hybrid films are very stable with no thickness reduction after a fewweeks.

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Mesoporous Zirconia Thin Films with Three-Dimensional Mesostructures

고영선, 권영욱

성균관대 화학과

We synthesized mesoporous zirconia thin films (MZTFs) by using a mixed solution in which zirconium hydroxide nanoparticles were self-assembled with amphiphilic block copolymers (ABCs). Those sol nanoparticles were prepared by refluxing ZrOCl2•8H2O and concentrated HCl in ethanol, and then characterized by using dynamic light scattering (DLS), X-ray diffraction (XRD), and energy-dispersive X-ray spectrometry (EDXS). These characterizations revealed that the sol nanoparticles were zirconium hydroxide with a hydrodynamic diameter in the range of 9–12 nm. To synthesize non-silica mesoporous materials, we should control not only the self-assembly properties of ABCs as templates, but also the condensation reactions of inorganic species. The self-assembly of ABCs 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 synthesized MZTFs in two steps: (1) the synthesis of zirconia hydroxide nanopaticles as presynthesized well-defined nanobuilding blocks (NBBs) and (2) the spin-coating technique with the solution mixed nanoparticles and ABCs in ethanol. This method involves several advantages. Among them, the processing parameters can be controlled more easily because the condensation of inorganic species can be suppressed during the self-assembly of ABCs due to the partially condensed nanoparticles. Consequently, we could synthesize MZTFs with highly ordered and 3-dimensional mesostrucutures as confirmed by small-angle X-ray scattering (SAXS), scanning electron microscopy (SEM), and transmittion electron microscopy (TEM). The 3-dimensional mesostructures of our MZTFs are very extraordinary results compared with other literatures in which 2-dimensional mesostructures (p6m) of MZTFs were reported only. Therefore, we expect that our MZTFs can be applied to a variety of fields such as electrochemical biosensors, optical devices, and membranes due to the accessible pores to the conducting substrate.

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Enhanced Perpendicular Magnetic Property of Epitaxial CoPt Nanoparticles by MSTF

김용태, 권영욱

성균관대 화학과

Magnetic recording is one of the most important research in ultrahigh density data storage. The research of patterned media and self-assembly of magnetic nanocrystal media in order to realize the ultrahigh density data storage has attracted attention as an important technology. The patterned magnetic media has to solved that the superparamagnetic limit for longitudinal recording on thin films occurring at the densities is about 200 Gbit/in2. The patterned medium is a promising candidate for the recording system with a capacity beyond 1 Tbit/in2. For example, a 25nm period patterned medium corresponds to a density of 1 Tbit/in2. However, in this approach, exist to solve the magnetic grains with size less than 25nm proplem. On the other hand, the self-assembly method of magnetic nanocrystal media can be smaller size and well arrayed. However, the perpendicular magnetic signal is unstable. Because dipolar interaction of particle-particle is more than magnetic field for smaller than few nanometer particles. Puntes et al. reported that the parallel hysteresis observed larger than perpendicular hysteresis in 12nm Co monolayer. This some limitation can be solved that the choice of large magnetic anisotropy (Ku) materials and the increase of interparticle spacing. Here, we tried arrays of CoPt quantum dot that are formed in the ordered mesoporous thin film by electrochemical deposition method. We applied a mesoporous silica thin film whose pore structure is composed of about 8 nm sized vertical channels and wall thickness is about 4nm sized in a hexagonal symmetry on the Au(111) surface as a nanoporous mask. We observed property of CoPt quantum dot that the epitaxial growth of (001) orientation on Au(111) surface, and the perpendicular anisotropy behavior by high-voltage electron microscopy(HVEM; JEM-ARM 1300S, 1250kV) and superconducting quantum interference device(SQUID).

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Effect of the poor solvent on the device efficiency of polymer solar cells deposited by spray processing

김미경, *유병관, **박두진, ***조장, ****김동유

*광주과학기술원 광공학응용물리학제 (PAP) *광주과학기술원 신소재공학과 **The commonwealth Scientific and Industrial Research Organisation Molecular and Health Technologies ***The university of california at santa barbara ****광주과학기술원 신소재공학과,나노바이오재료전자공학과*

Polymer solar cells (PSCs) can be fabricated by using various solution processes. Among these solution processes, the spray process is one of the most promising due to its high production speed, the application of a roll-to-roll system and large area fabrication, etc. In this presentation, we studied about the poor solvent effects on the spray deposition method for the PSCs. The principle of using the poor solvent is in order to control the aggregation of P3HT in mixed polymer- fullerene device active layers. Thus, we controlled the ratio of poor solvent to find the optimum ratio. There are notable effects in this study with using the poor solvent. Not only increase in crystallinity of P3HT but also decrease in surface roughness compared with spray deposited PSCs. Furthermore, the device performance is also improved due to the increase in the FF, Jsc and PCE values.

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Hollow sphere를 적용하여 결로방지와 실내공기질을 개선하기 위한 도료 개발

최정진, *황선

*한국건설생활환경시험연구원 신뢰성평가센터 *한국건설생활환경시험연구원 웰빙소재팀*

결로에 의한 집안에 서식하는 곰팡이는 불쾌한 냄새, 공기 중에 부유하는 곰팡이 포자로 인해 각종 피부, 호흡기질환의 직접적인 원인이 되고 있을 뿐 아니라, 정신적 피해는 시각, 후각적으로 불쾌한 실내 환경이 조성되어 한창 감수성이 발달하는 성장기 어린이와 중. 고등학생의 정신건강에 많은 악영향을 미친다. 또한 건축용 마감재에 대한 수요자 요구가 친환경성 추세를 보이고 있을 뿐 아니라, 정부 정책도 실내공기질 관리법 개정, 유해화학물질 관리법, 대기환경 보전법 및 친환경 도시건설(Eco-City)과 그린빌딩 인증제 도입 등 도료 관련 정책들이 환경친화형 도료의 적용을 필수적으로 요구하고 있어, 결로방지 촉매, 무기 충진제 및 무기 바인더를 적용하여, 결로방지, 난연 기능 뿐 아니라 항균, 소취 성능을 가지는 실내공기질 개선용 수용성 저온경화 무기도료를 개발하였으며 실내 환경 하에서의 결로 방지를 위한 세가지 mechanism 인 단열, 초친수성 및 흡습을 적용하기 위하여 단열소재인 hollow micro spheres (중심 입도 : 30~60 ㎛)와 초친수성 광촉매 소재 및 흡습 소재로 다공성의 규조토를 이용하였다.

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Synthesis and photovoltaic properties of Dye-sensitized solar cells using newly synthesized organic Dyes

조주열, *황도훈

*금오공과대 응용화학과 *부산대 화학과*

Dye-sensitized solar cells (DSSCs) have developed rapidly by many research groups because of their various advantages, such as high efficiency and low-cost devices for solar cells. Mainly DSSCs can divide with two parts, inorganic dyes and organic dyes. Inorganic dyes have been studied a lot and it gave also good results. For example Ru-polypyridyl-complex dyes, such as cis-dithiocy-anato bis(4,4`-dicarboxy-2,2`-bipyridine)ruthenium(II) (called N3 dye) can produce solar energy-to electricity conversion efficiency (è) of up to 11% under AM 1.5 G irradiation. Besides N3 dyes, metal-free organic dyes have been utilized in DSSCs because of their wide variety of the structures, facile modification, and high molar absorption coefficient. In this work we have designed and synthesized simple metal-free organic dyes for DSSCs and also have identified their photovoltaic properties.

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Patterned gold nanoparticles on the graphene

허성, 김승빈

포항공과대 화학과

In this study, new synthesized photoreactive gold nanoparticles were well-patterned in the graphene monolayer and its properties were modified by the nanoparticles. graphene is the most important materials in many field because it unique, remarkable properties. The application can be expanded by modification of its properties. Moreover, graphene-based nanomaterials have been intensively researched. Especially, the patterning process of nanomaterials on the graphene is the one of the important part.we fabricated well-patterned gold nanoparticles on graphene by photoreaction. These photoreactive gold nanoparticles can be patterned directly without photoresist and modified the properties of graphene monolayer. We suggest that this research can contribute to develop advanced graphene-based materials and its applications.

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Dissociative adsorption of oxygen molecule on nitrogen-doped graphene edge

김희진

KAIST EEWS

Formally the carbon materials, including nitrogen doped were well known to catalyze two-electron ORR(oxygen reduction reaction) and some mechanisms of it have been proposed. But in recent research from Matter et al, they proposed that nitrogen-doped carbon nanofiber can catalyze the ORR in four-electron pathway. And the nitrogen-doped carbon nanotube and graphene are also reported as to show four-electron electroreduction of oxygen even without transition metal present. However the four-electron reduction mechanism on the nitrogen-doped carbon materials is still unknown. In this study, we investigate the activation barriers and the dissociative adsorption energies of oxygen molecule on various types of graphene edges using density function theory calculations. Therefore we can understand the effect of edge and doped nitrogen to the dissociative oxygen reduction reaction.

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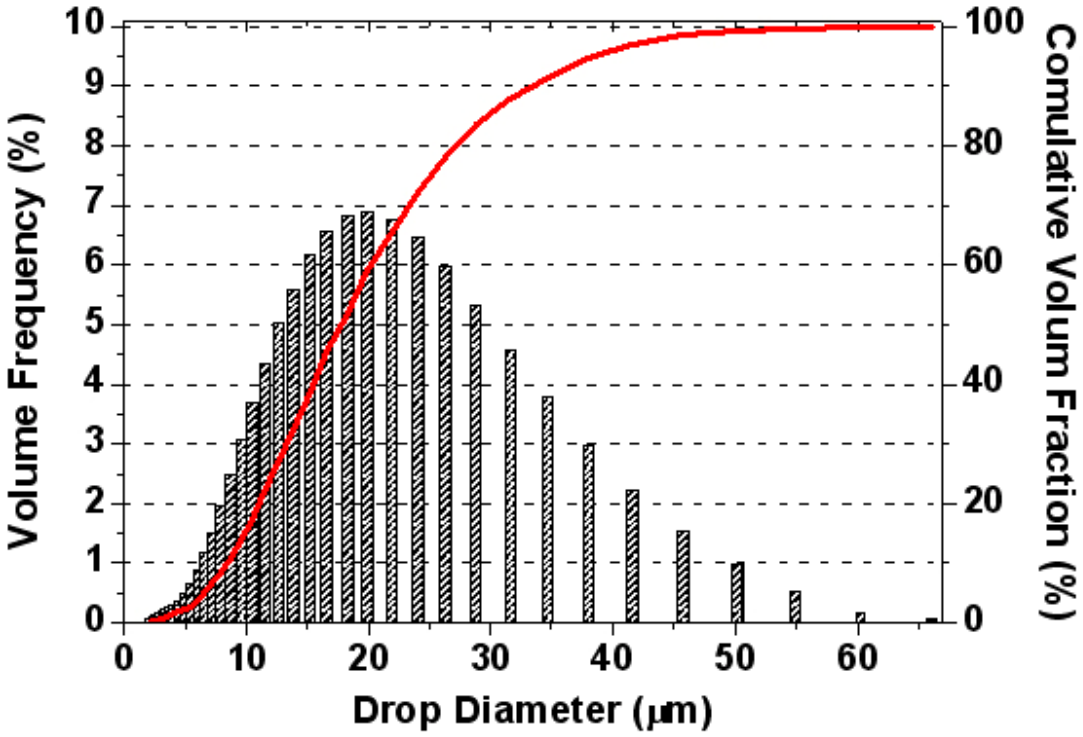
Factors to be Considered in Bulk Heterojunction Polymer Solar Cells Fabricated by the Spray Process

유병관, *박두진, **조장, ***김미경, ****김동유

*광주과학기술원 신소재공학과 *The Commonwealth Scientific and Industrial Research Organisation Molecular and Health Technologies **The University of California, Santa Barbara ***광주과학기술원 광공학응용물리학제 (PAP) ****광주과학기술원 신소재공학과,나노바이오재료전자공학과*

One of the attractions of solution-processed polymer solar cells (PSCs) is the potential for low-cost production by highthroughput roll-to-roll processes. The spray process can be suggested as an elegant alternative for PSCs fabrication due to its high production speed.We highlight the effects of sprayed droplet sizes on the film topography and drying time of droplets. We relate the latter to the PSCs device performances. The transfer efficiency and deposition rate of the spray process as a function of the droplet size are investigated for the high production speed and lowering the cost. PSC device fabrication with an optimized spray-operating condition yielded a power conversion efficiency of 3.4%. The comparable efficiency of PSCs fabricated by a roll-to-roll compatible process compared to spin-coated one achieved in this paper brings these devices one step closer to the realization of low-cost PSCs production.



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Preparation and characterization of core-shell structured silica@gold nanoparticles for control of surface plasmon resonance

배효선, 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 having silica core has been attractive not only because of its tuneable optical properties, but also its inertness in biological system. The monodispersed silica nanoparticles which is approximately 100 nm in diameter as a dielectric core were prepared by the Stöber method. The surface of silica nanoparticles was modified by 3-aminopropyltrimethoxy silane (APTMS). To obtain highly dispersed gold seed decorated APTMS-silica nanoparticles, the deposition-precipitation (DP) method was used. Through the systematic variation of pH, reaction temperature and time, homogeneously deposited gold nanocrystals on the surface of silica nanoparticles were obtained at pH 8 and reaction temperature at 65 ℃ for 45 min. Finally, silica@gold nanoshells with various shell thickness were prepared by following seed mediated growth method with various ratio of gold precursor and APTMS-silica nanoparticles. The size, morphology and elemental composition of the products were characterized by transmission electron microscopy (TEM), thermal analysis (TG-DTA) and fourier transform infrared spectroscopy (FT-IR). The optical properties of the gold nanoshells were analyzed by UV-vis spectroscopy.

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The Synthesis of Mesoporous Silica Thin Films (MSTFs) with Various Pore Diameters

이기림, 권영욱

성균관대 화학과

We report the synthesis of mesoporous silica thin films (MSTFs) with various pore diameters by using three different kinds of surfactants such as Brij-58, F-68, and F-127. Each of surfactants has different chain lengths, which determine the pore diameter of the mesoporous material. The pore diameters of the MSTFs synthesized by Brij-58, F-68, and F-127 were 2-3 nm, 5-6 nm, and 9-10 nm, respectively. The MSTFs were characterized by low angle X-ray diffraction (XRD), transmission electron microscopy (TEM), and scanning electron microscopy (SEM). Platinum nanostructured films were fabricated using the MSTFs as templates by electrodeposition method. The diameters of platinum nanorods were corresponds with the diameter of its templates. The surface enhanced Raman scattering effects of these platinum films were confirmed using Rhodamine 6G.

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Synthesis, crystal structure, and physical properties of a new semiconductor Bi2MnTe4

김태훈, *박철희

*(주)LG화학기술연구원 CRD *LG화학기술연구원 CRD 연구소*

Powder samples of Bi2MnTe4 have been prepared using a high-temperature reaction method; its structure has been determined via Rietveld refinement of powder X-ray diffraction data. The compound crystallizes in the trigonal space group R3m (Z = 3, a = 4.33 Å, c = 40.90 Å, and V = 664.86 Å3). Electrical conductivity and Seebeck coefficient measurements have been done in the temperature range of 50℃ to 400℃. Electrical conductivities of pressed pellets were found to be 125-130 S/cm at 325K. Variable-temperature Seebeck and electrical conductivity measurements revealed n-type semiconductor behavior.

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Carbon supported Pd_xPt electrocatalysts synthesized via sonochemistry towards formic acid oxidation

Matin Md Abdul, 권영욱, 장지훈

성균관대 화학과

A modified ethylene glycol-reduction method by ultrasound irradiation was developed to synthesize a series of Pd-enriched nanoparticle catalysts (Pd_xPt) with different molar ratios (1:1, 2:1, 3:1 and 4:1).These Pd-based catalysts were characterized by Transmission Electron Microscopy, Scanning Electron Microscopy-Energy Dispersive X-ray analysis, X-ray diffraction analysis and Cyclic Voltammetric method respectively to determine the average particle size, composition, surface morphology and electrocatalytic properties. The electrochemical activity of Pd-based catalysts was investigated in terms of formic acid electro-oxidation at low concentration in 0.1M perchloric acid at room temperature. Among catalysts, Pd_4Pt catalyst showed higher catalytic activity in formic acid electro-oxidation compared to that of others Pd-based catalysts, Pd-and Pt-catalysts. The result obtained from cyclic voltammograms indicates that Pd-based catalysts can be a promising candidate for anodic species in direct formic acid fuel cells. This method is very simple and has a great existing in possibility for mass-producing Pd-based catalysts as well as other noble metal catalysts.

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CVD grwoth of single-layer graphene on Ge surface

이재현

성균관대 나노과학기술학부

There have been great studies on 2-D graphene due to their potential application in nanoelectronics, optoelectronics and chemical sensors. Recently, using a transition metal such as Ni, Pt, Ru and Cu, high-quality graphene was synthesized by conventional chemical vapor deposition (CVD) method. However, transition metal as catalyst makes several problems for graphene electronics. Firstly, metal impurities induced deep-level defects which effects on the most electronic and optoelectronic devices. Secondly, perfect single layer graphene synthesis is impossible even we use Cu catalyst. Here, we report a novel approach to CVD growth of single layer graphene on Ge surface. Since solid solubility of carbon in Ge is negligible at growth temperature, nearly 100% of area is converd by single lyaer. This growth approach serves an important point for future graphene nanoelectronic devices.

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Facile Preparation of Carbon Supported Co-Pd Alloy and Core-Shell Nanoparticles by Ultrasound and Their Enhanced Electrocatalytic ORR Activity

장지훈, 권영욱

성균관대 화학과

Carbon supported Co-Pd nanocomposites with different surface structure and various ratio of Co/Pd were synthesized by ultrasound assisted polyol process. Sonochemical treatment of palladium acetylacetonate and cobalt acetylacetonate in ethylene glycol in the presence of a carbon support without any other surfactant, reagent for pH adjustment or stabilizer produced 4-7 nm sized CoxPd nanoparticles dispersed on the carbon support. The absence of additional reagents in the sonochemical reaction system makes unsoiled nanoparticles in comparison with conventional wetting methods. The structures of the nanoparticles, pure Pd, Co-Pd alloy and core-shell structures were characterized by XRD and TEM. Electrocatalytic oxygen reduction reaction (ORR) behavior of the materials was measured by rotating disk electrode (RDE) method and compared with pure Pd/C and commercial Pt/C. We obtained a larger mass activity for ORR with Co-Pd mixed phase samples than pure Pd/C and a comparable result with commercial Pt/C. Especially, Co0.25Pd core-shell structure shows a remarkable enhanced activity for ORR.

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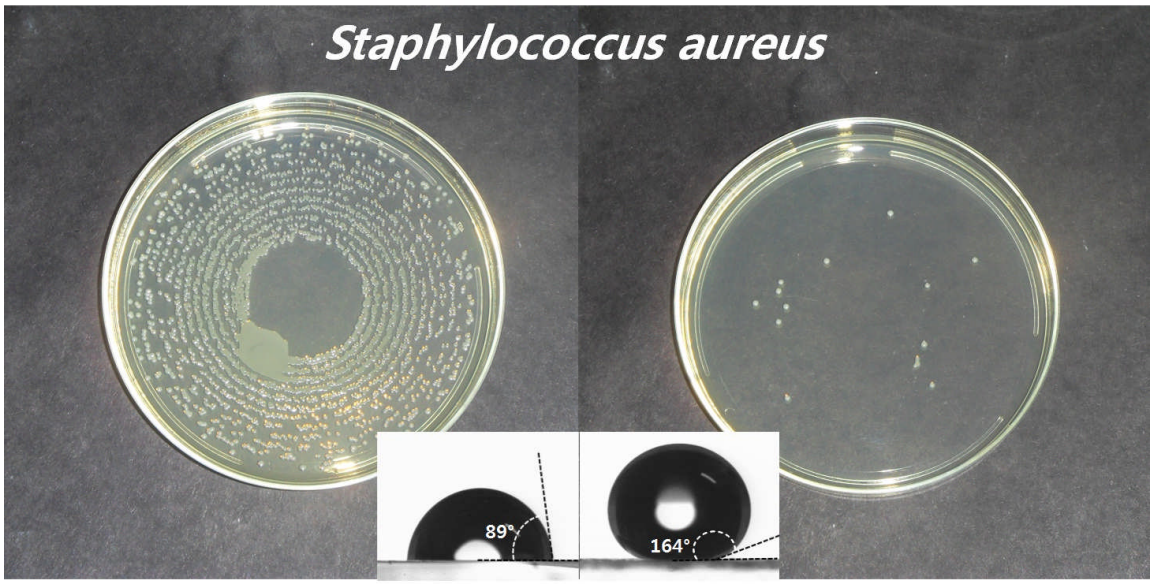
Simple and facile technique to prepare superhydrophobic surface coatings with anti-bacterial properties

윤종해, *Benjamin J. Privett, *Mark H. Schoenfisch, 신재호

*광운대 화학과 *Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA*

Superhydrophobic surface coatings with high static water contact angles (>150°) have received tremendous attention in recent years. The applications of superhydrophobic coatings are diverse due to their unique water-repellency, self-cleaning ability, and anti-biofouling property. A variety of strategies to fabricate superhydrophobic surfaces have been reported including surface roughening, chemically lowering the surface free energy, lithographic patterning, laser/plasma etching, and vertical alignment of nanostructured materials. These coating materials, however, typically require harsh synthetic conditions and/or complicated fabrication techniques, and possess poor substrate compatibility. Herein we demonstrate a simple and facile synthesis of superhydrophobic surface coatings composed of silica particles immobilized in a perfluorinated xerogel film. The surface coatings prepared in this work are characterized in term of water contact angles, surface roughness, and physical stability. Furthermore, to evaluate anti-biofouling propensity, the coatings are exposed to bacterial solutions (i.e., 108 cfu/mL of Pseudomonas aeruginosa and Staphylococcus aureus) under flowing conditions.



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Fabrication of $CuInSe_2$ Thin Film Using Non-Vacuum Solution Deposition Technique

조정민, 배은진

한국전자통신연구원 창의연구본부/융합기술원천연구팀

$CuInSe_2$ thin films were prepared successfully with the chemical spray pyrolysis as a function of Cu/In atomic ratios and variation of selenium contents. The X-ray diffraction, UV-visible spectroscopy, the Hall effect measurement and scanning electron microscopy were carried out for the compositional and structural analysis. The effects of the Cu/In ratio and selenium concentration were observed in the XRD, SEM, UV-visible spectrum and the Hall effect measurement analysis for fabricated thin films. The XRD and UV-visible analysis results showed an increase or decrease of crystallinity and shift of transmittance tendency depending on the copper and selenium content. The thin film grain size was increased with the increase of copper content. In the thin films, the variation of Cu/In ratios between 0.8 to 1 showed an increase on hole density, but a decrease of Hall mobility and resistivity. We suggest the formation of CuxSe phase particles or layers depends on the spray solution. Based on these results, we will fabricate and characterize CISe/CIGSe thin film solar cells in further work.

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A New Platform for enhanced siRNA Delivery based on Gold Nanoparticles

유수윤, 장홍제, 민달희

KAIST 화학과

Gold nanoparticles are inorganic nanoparticles which possess unique 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 with various diameters 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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In vivo Molecular Imaging of Cancer using Gold Nanoparticle Probes functionalized with 125I and cyclic RGD-PEG

홍수현, 남좌민

서울대 화학부

We designed and synthesized 13 nm gold nanoparticles which are PEGlyated and functionalized with cyclic RGD for targeting cancer cells. These probes were labeled with 125I by electrostatic interaction. 125I-labeled cyclic RGD-gold nanoparticle-probes show high stability in high salt and temperature conditions and high specificity for integrin αvβ3 expressing cells (U87MG).αvβ3 expressing human glioblastoma cancer cell (U87MG) and non-expressing breast cancer cell (MCF7) were treated with 125I-echistatin as the integrin αvβ3-specific radioligand in competitive binding assay with cyclic RGD-gold nanoparticles and cyclic RGD peptides. The IC50 values obtained from this competitive binding assays were 2.17 nM for cyclic RGD-gold nanoparticles and 154 nM for cyclic RGD peptides. MCF7 cells showed the same uptake efficiency for both cases. To determine internalization of cyclic RGD conjugated gold nanoparticles, TEM images of U87MG and MCF7 were acquired and they showed intracellular localization of the probes only in U87MG cells but not in MCF7 cells. Cell viability assay results showed that these probes have no cytotoxic effects upto 500 μg/ml probe concentration and 72 h incubation for both U87MG and MCF7 cell lines. The uptake and clearance of 125I-labeled cyclic RGD-gold nanoparticles in vivo was evaluated by serial SPECT/CT studies in a U87MG tumor bearing mouse using a dedicated small animal SPECT/CT system. These in vivo imaging results (Figure 1) showed high uptake of the probes in the U87MG xenografted tumor and blood pool up to 1 h post-injection and also showed clearance of these probes from the body by renal and urinary excretion > 1 h after injection. In this study, we demonstrated that 125I-labeled cyclic RGD-gold nanoparticles can define αvβ3 expressing cancer cells both in vitro and in vivo. These probes may have a potential in tumor and angiogenesis targeted imaging technique which will be useful for various diagnostic and therapeutic applications.

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Printable carbon free CIGS thin film for solar cell applications

박세진, *민병권

*고려대 화공생명공학과 *KIST 청정에너지연구센터*

$CuIn_xGa_{1-x}(Se_yS_{1-y})_2$(CIGS) thin film solar cell has been considered to one of the most promising ways to convert sunlight into electrical energy due to its high efficiency as well as high durability. The obstacles of the CIGS thin film solar cell fabrication for commercial applications may be relatively difficult manufacturing synthetic method and high processing costs because it is conventionally fabricated by a vacuum based deposition technique. Herein, we suggest a simpler and lower cost synthetic method of CIGS thin film by applying a paste coating methode. In this method the paste containing Cu, In, Ga precursor mixtures was firstly prepared followed by being printed on conducting glass substrates. The film was then annealed at three different conditions: an annealing at 450 ^oC in ambient atmosphere, an annealing at 500 ^oC in H_2S/Ar atmosphere, and an annealing at 500 ^oC in Se vapor. The stoichiometric CIGSSe film was synthesized with the film thickness of ~2μm. Importantly, almost no impurity of carbon and oxygen was found in the CIGS film which would be very beneficial in solar cell applications. The compositional and structural characteristics of the film were investigated by various analysis techniques including XRD, SEM and EPMA, and will be discussed in the presentation.

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Synthesis of chalcopyrite nanocrystal inks by a solvothermal route for CIGS thin films

조진우, *김웅, **민병권

*고려대 신소재공학과 *고려대 신소재공학부 **KIST 청정에너지연구센터*

Non-vacuum processes such as printing, electroplating and spraying have been suggested to solve the high cost problems of the current vacuum based $Cu(In_xGa_{1-x})Se_2$ (CIGS) solar cell fabrication methods. Particularly, the printing method using a nanocrystal ink would be the most promising considering manufacturing cost and large panel fabrication. In this study, in order to achieve the printable CIGS thin films, chalcopyrite copper indium sulfide ($CuInS_2$), copper indium selenide, and copper indium gallium selenide ($Cu(In_xGa_{1-x})Se_2$) nanocrystals were synthesized by an arrested precipitation in solution. These nanocrystals were then re-dispersed in organic solvent with a suitable viscosity to use as an ink. After drop casting and annealing the films were sulfurized and/or selenized in H_2S/Ar and/or Se vapor environment, respectively. The structural and optical properties of the chalcopyrite nanocrystals and films will be discussed in the presentation.

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Fabrication of TIPS-Pentacene Single Crystal Nanowires by using Nano-transfer Molding

오현석, 성명모

한양대 화학과

In recent years, organic thin film transistors OTFTs based on conductive-conjugated molecules have received significant attention and pentacene is the most promising organic semiconductors. However pentacene has insolubility in organic solvents so pentacene OTFTs can be achieved with vacuum evaporation system. However 6, 13-bis (triisopropylsilylethynyl) (TIPS) pentacene has high solubility in organic solvent that reported by Anthony et al. Furthermore, the substituted rings in TIPS-pentacene interrupt the herringbone packing, which leads to cofacial π-π stacking.We report a fabrication of TIPS-pentacene single crystal nanowires that made on Si substrates by liquid bridge-nanotransfer molding (LB-nTM) with polyurethane acrylate (PUA) mold. LB-nTM is based on the direct transfer of various materials from a stamp to a substrate via a liquid bridge between them. In liquid bridge-transfer process, the liquid layer serves as an adhesion layer to provide good conformal contact and form covalent bonding between the TIPS-pentacene nanowire and the Si substrate. The patterned TIPS-Pentacene single crystal nanowires have been investigated by Atomic force microscopy (AFM), Transmission Electron Microscopy (TEM), X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and electrical properties.

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Growth of single crystalline germanium/carbon-core/shell nanowires

김병성

성균관대 성균 나노과학기술원

Recently, germanium nanowires (GeNWs) have attracted much attention due to their unique one dimensional nanostructure, the advanced electrical properties such as high carrier mobilities, and compatibility with existing IC process. Various growth mechanisms for single crystalline GeNWs until now. Among them, VLS growth method by transition metal catalyst has been much widely used because it provides a facile route for synthesis and allows to control the morphology and doping ratio during the growth process. However, conventional GeNW growth by VLS method has many problems, such as metal impurities contamination, and ununiform dopant and Ge adsorption on NW side wall. In addition, more fundamental issue is that Ge easily forms unstable oxides on the surfaces. Compared with chemically and electronically stable Si/SiO_2interface, the Ge/GeO_xinterface has considerably high surface states and is trouble with unfavorable electrical properties and poor chemical instability. Herein, we present single crystalline germanium nanowire growth with protective carbon shell by low-pressure chemical vapor deposition (LPCVD) process. Carbon shell has amorphous nanostructure with very thin thickness of 2-3nm. It can be acted as not only the passivation layer preventing the oxidation at even high temperature, but also barrier for metal diffusion during GeNW growth process. In addition, the simultaneous shell growth prevents the uncatalyzed Ge deposition. These carbon shell effects on NW growth were investigated using field emission scanning electron microscopy (FE-SEM), raman spectroscopy, and high resolution transmission electron microscopy (HR-TEM).

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Synthesis of CIGS nanoparticle and thin films by Non-Vacuum Deposition Methods

배은진, 조정민

한국전자통신연구원 창의연구본부/융합기술원천연구팀

The CIGS (Cu(InGa)Se2) thin films were successfully synthesized by using non-vacuum deposition methods. Those methods were nanoparticle-precursor deposition and non-vacuum spray deposition. The synthesized CIGS thin films had typical characteristics of CIGS for absorber layer. The structures of CIGS thin films were chalcopyrite and the properties of thin films were dense and smooth. The microstructure of CIGS thin films were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), uv-vis spectroscopy. We could grow chalcopyrite CIGS absorber layers with high dense and large faced grains. We suggest the potential use of these processes for low cost and high quality solar cell fabrication.

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Preparation and characterization of in-situ anchored Pt NPs into frameworks of mesoporous silica

이형석, *정진국, **유중환

*한양대 화학공학과 *고려대 화공생명공학과 **한국세라믹기술원 에코복합소재센터*

The metal catalysts, usually dispersed as nanometer-sized particles on supports with high surface area, are subject to sintering or coalescence to minimize their surface energies through the Ostwald ripening process. This results in a decrease in the amount of surface atoms in metal nanoparticles and a consequent loss of catalytic activity. Several strategies towards stabilization of nanometer-sized metal particles against the sintering problem have been pursued, including design of metal/metal oxide core-shell nanostructures, addition of stabilizing metal oxides, and use of sintering-resistant supports. Here, we present an improved method to synthesize an in-situ anchored Pt NPs into the frameworks of the sulfur-containing mesoporous silica (SMS) through co-condensation method. The Pt NPs well dispersed and anchored into the frameworks of the SMS are enough stable to be recycled multiple times.

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Efficient siRNA delivery system in vitro and in vivo based on pore expanded silica nanoparticle

나희경, 민달희, 김미희, 유수윤

KAIST 화학과

RNA interference (RNAi) is an evolutionarily conserved biological process in which a double stranded RNA inhibits gene expression by degrading target mRNA or by blocking the translation pathway of a specific gene. The application of RNAi using siRNA (small interfering RNA) in biomedical area might have great potential to treat diseases that cannot be treated by conventional small molecule drug. Mesoporous silica materials appear to possess immense potentials in catalysis, biosensors and drug delivery systems due to tunable pore and particle size, high surface area, large pore volume, and biocompatibility. In particular, monodispersed silica spheres with large pores are very important for the incorporation of large molecules such as metal complexes and proteins into mesopores, and for the retention of pore space after grafting of organic functional groups. Here, we report an efficient siRNA delivery system based on pore expanded silica nanoparticle. It is shown that newly developed siRNA delivery system is novel and powerful gene delivery vehicle in vitro and in vivo. Our study demonstrates that siRNA-pore expanded silica nanoparticle complex can serve as potential gene silencing therapeutics for treating various diseases.

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A New Platform for Endonuclease Activity Assay Based on Graphene Oxide

이지언, *김미희, *민달희

*KAIST 화학과 *KAIST 화학과*

Endonucleases, a family of nucleases that can hydrolyze the internal phosphodiester bonds in DNA or RNA, are one of the most important enzymes in molecular biology. Among them, restriction enzyme(type Ⅱ) used in the laboratory for DNA analysis and gene cloning cut DNA at defined positions close to or within their recognition sequences. Therefore, assay of restriction enzyme activities and evaluations of the kinetic parameters are valuable in the fields of clinical diagnostics, drug discovery, and nanoscience. Currently, the detection methods have included gel electrophoresis, high-performance liquid chromatography (HPLC), filter binding, and enzyme-linked immunosorbent assay (ELISA). Although extensively used, the above-mentioned assays suffer from serious disadvantages. They are time consuming and generally not quantitative. Moreover, many assays only allow for a discontinuous detection of DNA cleavage, because the cleavage products must be separated from the substrate.Herein, we describe a new restriction activity assay method based on the difference of binding affinity between single stranded DNA and double stranded DNA with graphene oxide(GO). The substrate DNA of the enzyme consists of single and double strand part containing recognition site. By measuring the quenching and recovery of fluorescence of dye conjugated to double strand part, restriction enzyme activity can be assayed. This GO-based method allows real-time measurement and quantitative assay of restriction enzyme in short time. We believe that this new GO based restriction enzyme assay platform will be a widely applicable tool in endonuclease related basic research and drug development.

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Fabrication of LaPO4:Eu thin films by SILAR method

박동호, *박상문

*인제대 의생명화학과 *신라대 에너지응용화학과*

Thin films of Eu-doped LaPO4 were fabricated on glass substrate using a successive-ironic-layer-adsorption-and-reaction (SILAR) method and subsequent hydrothermal and/or furnace annealing. X-ray diffraction patterns exhibit the phase transform from hexagonal LaPO4 in as-prepared film to monoclinic in hydrothermal and/or annealing. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images of LaPO4:Eu show the homogenous morphology of micro-sized nanofibers around 10 to 20 nm in diameter. The red LaPO4:Eu phosphors activated at 254 nm are discussed.

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Application of Porous Silica Nanoparticles with Large Pores in Gene Delivery

김미희, 나희경, 김영관, 유수윤, 민달희

KAIST 화학과

Gene therapy using nanoparticle platform offers great promise for treatment of cancer and genetic disorders. The considerations of the nanoparticles to be used as drug carriers are ease of cellular uptake, gene expression efficiency, gene loading capacity, and biocompatibility. Silica nanoparticle has been attractive candidate as gene delivery vector because of several advantageous features such as facile synthesis and modification, stable porous structures, large surface areas, low cytotoxicity, and encapsulation of drugs and genes.In this report, we used expanded porous silica nanoparticles (EX-SiNP) with large pores for gene delivery system. This particle was aminated to hold pDNA through electrostatic interaction, and conjugated with TAMRA dye for imaging. Enough positive charges of particle according to the large surface area made possible to transfect into cells efficiently and have high loading capacity of pDNA. Moreover, in contrast to the conventional methods which require cationic lipids or polymers as supplementary materials, the present system doesn't need to be supported by any polymers or lipids. We believe that this system contributes to the growth of the efficient drug delivery system and diagnostic tools due to considerable possibility of further applications such as siRNA delivery, large peptide/protein delivery, and highly sensitive biosensors.

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Graphene Oxide/Multi-Walled Carbon Nanotube Double Layer Films as a Novel Platform for Laser Desorption/Ionization Mass Spectrometry

김영관, 곽설진, 나희경, 유수윤, 홍승희, 홍승우, 민달희

KAIST 화학과

Matrix-assisted desorption/ionization mass spectrometry (MALDI-MS) MALDI and Imaging mass spectrometry (IMS) have become powerful tools for biochemical analyses, pharmacology and proteomic researches due to its high sensitivity and accuracy. Although MALDI-MS and IMS have been successful in analyzing varieties of molecules with molecular weight of 1 to 100 kDa and tissue imaging, the addition of organic matrix molecules have resulted in several problems such as interference in low mass-region (m/z

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Reduction of 4-nitrophenol Catalyzed by Various Metal(Pt, Au, Ag) Nanoparticles Embedded into Carbon Nanocolloids

이정호, 홍성규, 고원배

삼육대 화학과

The synthesis and characterization of catalysts based on the nanomaterial supported on carbon nanomaterial for the reduction of 4-nitrophenol was investigated. Metal(Pt, Au, Ag) nanoparticles were deposited on the surface carbon nanocolloids in the aqueous solution. The reduction of 4-nitrophnol in aqueous solution with metal(Pt, Au, Ag) nanoparticles which were embedded into carbon nanocolloids have been studied by UV-vis spectra and LC-MS. The fabricated metal(Pt, Au, Ag) nanoparticles decorated carbon nanocolloids showed better catalytic performance of 4-nitrophenol reduction than the corresponding only metal nanoparticles. Carbon nanocolloids performed as a supporter on the homogeneous dispersion of metal nanoparticles in the aqueous solution. The order of catalytic effect as the same mole concentration of the various metal(Pt, Au, Ag) nanoparticls was of the following things; Pt > Au > Ag. The nature of nanoparticles decorated carbon nanocolloids were characterized by X-ray diffraction(XRD) and transmission electron microscopic(TEM) analysis.

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Surface-Enhanced Raman Scattering of Graphene and Interaction between Metal and Graphene

이지숙, 신현석

울산과학기술대 에너지공학부

Surface-enhanced Raman scattering (SERS) of graphene on SiO_2 (300 nm)/Si substrate was investigated by depositing Au & Ag nanoparticles using thermal evaporation. When Au & Ag nanoparticles were deposited on the graphene, the G band was enhanced 120 times for Au deposition at 633 nm excitation and 24 times for Ag deposition at 532 nm excitation in single-layer graphene. Single-layer graphene provides much larger SERS enhancement compared to few-layer graphene, while in single-layer graphene the enhancement of the G band was larger than that of the 2D band. After metal nanoparticles deposition, asymmetric G band was observed. The asymmetry of G band is larger in single-layer graphene than in few-layer graphene. Lastly, to elucidate multiple reflections between the Si substrate and deposited metal nanoparticles, a transparent glass substrate was used for measuring SERS enhancement of graphene. The contribution of multiple reflections to total enhancement on the SiO_2 (300 nm)/Si was 1.6 times out of average SERS enhancement factor, 71 times.

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rGO wrapped fullerene (C_{60}) wires

양지은

울산과학기술대 에너지공학부

The assembly of reduced graphene oxide (rGO) and fullerene (C_{60}) into core/shell hybrid wires was successfully performed by employing the liquid-liquid interfacial precipitation (LLIP) method. C_{60} wires are first formed and then rGO sheets are coated on surfaces of them. The structural characterization of the rGO/C_{60} wires was carried out by using UV-Vis, SEM and HR-TEM. FET devices with rGO/C_{60} wires were prepared to investigate their electrical properties. The I-Vg curve of the hybrid wires exhibited a p-type semiconducting behavior at room temperature, indicating hole transport through rGO as a shell layer. Furthermore, we showed interesting applications using the hybrid wires: photocurrent generation and solar cells.

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Epidermal growth factor receptor targeted cancer destruction by combined chemotherapeutic and photothermal therapy with single-walled carbon nanotube

문혜경

포항공과대 화학과

Selective targeting is an important approach with great potential for overcoming challenges associated with adverse effect and poor effectiveness in cancer treatment and drug delivery system. Nanomedicine recently plays a pivotal role in cancer therapeutics by specific targeting to the cancer cells thereby improving effectiveness and reducing systemic toxicity. We developed cancer targeted therapeutic agent with single-walled carbon nanotube (SWNT). On the advantage of its unique physicochemical properties and good biocompatibility, SWNT can be served as a good nanoscale vehicle for therapeutic purpose. For selective targeting and destructing of cancer cells, we functionalized SWNT with cetuximab as a targeting moiety, lapatinib as a anti-cancer drug and Cy5.5 as a imaging agent. The Cy5.5-Cetuximab-SWNT conjugate was synthesized by EDC/NHS coupling chemistry and characterized by colorimetric, microscopic and spectroscopic method. The specific reactivity to epidermal growth factor receptor (EGFR) of this conjugate was evaluated by flow cytometry and fluorescence microscopy. In vitro cytotoxicity efficiency of this conjugate was achieved in combination with noninvasive exposure of near infrared light (NIR). The cellular incubation of this conjugate showed the high affinity to EGFR positive cancer cell and inhibition of cell proliferation as well. This result provides general approach for selective therapeutic treatment of various type of EGFR overexpressed cancers.

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Novel PL emission enhancement of M-ABA(M=Znic and Cobalt) complex

Min Yu lin

포항공과대 화학과

Novel M(M=znic or cobalt)–m-Aminobenzoic Acid complexes have been successfully synthesized by a simple refluxing reaction using M(acetate) and m-Aminobenzoic acid for the precursors. The formation processes of the morphologies and the superstructures of the complexes were proposed based on the time-dependent evolution process. This new complexes show huge PL emisssion enhancement in the near-UV region (410nm) compared with pure m-ABA. On the other side, the metal complexes enables excited state intramolecular proton transfer (ESIPT), giving an additional emission band in the near-IR region (800 nm) with a large Stokes shift.This approach opens a new and effective way for the fabrication of amino acid hybrid materials with unique optical properties and is expected to allow access to other organic/organic hybrid materials with structural specificity and functional novelty.

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AMPEROMETRIC SENSOR BASED ON MONOLAYER PROTECTED Au_{25}CLUSTERS

S. Senthil Kumar, *곽규주, *이동일

Department of Chemistry Yonsei University *연세대 화학과

Much effort has been made to develop sensitive and selective methods for the determination of biologically and environmentally important compounds as these compounds show great diversity and analytical complexity. The development of chemically modified electrodes (CMEs) is an emerging field in electrochemistry with an objective of lowering the oxidation potentials of selected important analytes and enhancing the selectivity in the electroanalytical methods, due to the selective interaction of the electron transfer mediator with the target analyte. Monolayer protected gold clusters (MPCs) are new materials with numerous possibilities in electrocatalysis and amperometric detection since they are composed of very few atoms, with a core size in the sub-nanometer regime, and the ligands can be engineered easily facilitating in improved sensitivity and selectivity. In the present work, we have synthesized Au_{25}MPCs and utilized them for the first time in the electrocatalytic oxidation and amperometric detection of some biologically and environmentally significant analytes such as ascorbic acid, dopamine, sulphite and hydrazine. Au_{25}MPCs have been synthesized using the modified Brust-Schiffrin method. The synthesized particle had shown absorbances at around 320, 395, 436 and 665 nm, characteristic of Au_{25}MPCs. The particle size estimated from the TEM studies is found to be 1.1±0.2 nm, corresponding to that of Au_{25}MPCs. Au_{25}MPC modified electrode has been fabricated by entrapping gold nanoparticles into a thiol-containing sol-gel network. The cyclic voltammogram of the modified electrode exhibited well-defined redox peaks with a formal potential of 0.26 V in 0.1 M KCl at a scan rate of 0.1 Vs^{-1}. The modified electrode has shown excellent catalytic activity towards the electrochemical oxidation of the above mentioned analytes. The catalytic currents were found to vary linearly with the concentration of the analyte added, based on which a calibration graphs have been obtained. Hydrodynamic

voltammetry and chronoamperometric studies revealed the utility of the modified electrode in dynamic conditions.

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Investigation of Al Oxide Film using Frequency Impedance Measurement in Borate Buffer Solution

김현철, 김연규

한국외국어대 화학과

Borate 완충 용액에서 양극 산화에 의해 생성되는 Al 산화 피막의 생성 과정과 이 피막의 전기적 특성을 단일 주파수 기법과 다중 주파수 기법을 이용하여 조사하였다. Al 산화 피막은 주로 Al_2O_3로 구성되어 있으며, n 형 반도체의 전기적 성질을 보였다.

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Investigation of Surface Renewable Graphene Paste Electrodes for Electrochemical Sensing

우승희, 김양래, 정택동, *박원철

*서울대 화학부 *서울대 융합과학기술대학원 나노융합학과*

A new carbon electrode material, obtained by mixing graphene with a mineral oil binder was studied. Graphene was synthesized by modified Hummer's method. Transmission electron microscopy, x-ray diffraction, scanning electron microscopy, and Raman spectroscopy clearly demonstrate that graphene was successfully synthesized. The electrochemical behavior of graphene paste electrodes was compared with that of graphite paste electrodes and multi-wall carbon nanotubes paste electrode. Several redox species, such as $Fe(CN)_6^{3-/4-}$, dopamine and ascorbic acid, were used to probe the electrochemical properties of these graphene paste electrodes by using the cyclic voltammetry, differential pulse voltammetry, and electrochemical impedance spectroscopy. The graphene paste electrodes demonstrate fast electron transfer kinetics and possess excellent electrocatalytic activity.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Flexible multi-color electrochromic film devices based on Prussian blue analogues

정영희, 권기범, 박승욱, 곽준영, 김영일

부경대 화학과

Electrochromic devices can be changed color by applied a small voltage. It means that the amount of light and heat passes through the devices can be controlled. So We can use them as energy-saving devices.Prussian blue(PB, iron(Ⅲ) hexacyanoferrate(Ⅱ)) is a well-known electrochromic material and its analogues with the Fe ions replaced by various combinations of transition metals show electrochromic properties.We synthesized nano sized Prussian blue analogues particles such as Cu-PB, Co-PB and Ni-PB, characterized by XRD, TEM, SEM, UV-vis spectrometer and Cyclic voltammetry.For lower manufacturing cost of electrochromic device and diverse application, We used sol-gel technique, it is simplified method of preparing a uniform film with large area, and coated on ITO/PET.PB/Ni-PB, PB/Cu-PB, PB/Co-PB devices were tested long-term stability for the practical usage, showed good stability, high contrast ratio and short response time.

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Hydrogen production in single chamber microbial electrolysis cell using PANI-nano fiber fabricated bio-cathodes

전용원, Ahmed Jalal, *김성현

*건국대 생명공학과 *건국대 특성화학부생명공학과*

Microbial electrolysis cells (MECs) provide a new approach to hydrogen production through the electrohydrogenesis. Hydrogen gas can be generated from biodegradable organic matters such as acetate, glucose in MECs. Evolution of hydrogen by microbial electrolysis usually requires precious metal catalysts such as platinum (Pt) on the cathode for the proton reduction. In order to achieve hydrogen production without using Pt, polyaniline (PANI)-nano fiber fabricated biocathodes have been employed. At an applied voltage of 0.8V and by using acetate as a substrate, the hydrogen production rate of 1.96 m^3/m^3/day was achieved, which was slightly lower than that with Pt cathode.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Removal of Hg^{2+} as an electron acceptor with power generation using a microbial fuel cell

최찬수

대전대 응용화학과

In this study, removal of Hg^{2+} coupled with power generation was attempted by using Hg^{2+} as an electron acceptor in a microbial fuel cell (MFC). The initial pH affected the removal efficiency of Hg^{2+} from electrochemical and chemical reactions. The effluent Hg2+ concentrations after a 5-hour reaction were 3.08 ± 0.07, 4.21 ± 0.34, 4.84 ± 0.00, and 5.25 ± 0.36 mg/L for initial pH levels of 2, 3, 4, and 4.8, respectively. For 10 hours of reaction, the calculated effluent Hg concentration was in the range of 0.44 - 0.69 mg/L. Up to 99.56% Hg2+ was removed and the effluent concentration was 0.44 mg/L after 10 hours for the initial Hg^{2+} concentration of 100 mg/L at pH 2. Both initial pH and Hg^{2+} concentration, affected power generations. A maximum power density of 433.1 mW/m^2 was achieved from 100 mg/L Hg^{2+} at pH 2.

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발표분야: 전기화학
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Improvements in Nafion Membrane Performances in PEMFCs with Biopolymeric Multilayers

남은지, *이재영, 이혜진

*경북대 화학과 *광주과학기술원 환경공학과*

Nafion membranes are one of the most widely used as a reference material in polymer electrolyte membrane fuel cells (PEMFCs) because of good proton conductivities and chemical stabilities below 100℃. However, there has been a great demand to improve the performance of Nafion film in fuel cell applications with respect to water swelling, fuel cross-over as well as proton conductivities. In this poster, we demonstrate a simple layer by layer (LbL) assembly method for creating biopolymeric electrolyte layers on a conventional Nafion membrane to enhance the membrane performance in PEMFCs. The biopolymeric electrolyte multilayers on a negatively charged Nafion membrane were formed via the electrostatic adsorption of alternating oppositely charged layers, namely poly-L-lysine as a positive layer and DNA as a negative layer. Various thicknesses of biopolymeric multilayers assembled on a Nafion membrane were investigated for three different measurements including proton conductivities, water uptake rates and swelling rates. Our preliminary data show that the use of biopolymeric electrolyte multilayers on a Nafion membrane can reduce the swelling phenomena of the membrane as well as enhance proton conductivities of the membrane.

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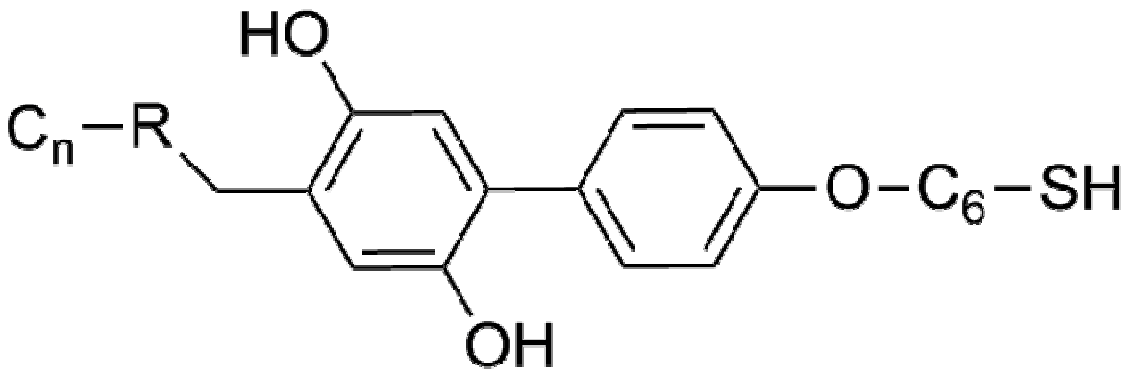
End-Group-Dominated Electrochemical properties of Hydroquinone Self-Assembled Monolayers on Gold

박원철, 김성현

건국대 특성화학부생명공학과

The self-assembly and electrochemical properties of a new class of thiol-functionalized hydroquinone derivatives were studied on gold electrodes by cyclic voltammetry. The compounds (referred to as Cn-R-CH2-H2QC6SH SAMs (R = O and NH, n = 4, 10, and 16) were synthesized and characterized. They spontaneously adsorb onto a gold surface to form stable and reproducible monolayers. The Cn-R-CH2-H2QC6SH SAMs (R = O and NH, n = 4, 10, and 16) showed well-behaved voltammetric responses in aqueous solution that corresponded to a two-electron, two-proton reduction/ oxidation of the hydroquinone redox center. In this presentation, end-group-dominated electrochemical properties of hydroquinone self-assembled monolayers on gold will be discussed in detail.



R = O, NH
n = 4, 10, and 16

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발표종류: 포스터, 발표일시: 목 15:00~17:00

A menadione/carbon powder composite modified anode for power enhancement in single chamber microbial fuel cells

Ahmed Jalal, 박원철, 김성현

건국대 특성화학부생명공학과

Modification of anode with different materials has been proven to be a successful alternative for the improvement of power generation in the microbial fuel cells (MFCs). A new approach of improved performance of MFCs with the use of menadione/carbon powder composite modified anode is explored in this study. The immobilization of redox active menadione accomplished by mixing with carbon powder and Nafion binder applied on the carbon cloth. Menadione formal potential is negative enough to easily accept electrons from the outer membrane cytochromes of microorganisms that can directly interact to the solid surface. Its properties help to accelerate electron transfer process from the bacteria to the anode. A single chamber air cathode MFC inoculated with aerobic sludge gave maximum power of 1250 mW/m^2, which is 30% higher than that of unmodified anode, showing a positive effect of menadione mediated electron transfer to the anode surface.

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Porous 2-dimensional dimethylglyoxime monolayer on Au(111)

김혜란, 김세철, *김혜령, *정창훈, *김잔디, 김영래, *이충균

*충남대 분석과학기술대학원 *충남대 화학과*

Au(111)과 같은 고체 표면에 형성된 유기 박막층은 일정한 패턴의 단분자 박막층으로, 3 차원 구조체 형성의 template 로 활용될 수 있다. 이러한 관점에서 새로운 template 로서의 가능성을 검토하기 위하여 dimethylglyoxime (DMG)분자의 분자간 수소 결합을 이용한 template 형성을 STM(Scanning tunneling microscope)으로 관찰하였다. STM 관찰결과, Au(111) 표면 전체에서 두 가지의 2 차원 network 를 관찰할 수 있었다. 하나는 ($2\sqrt{3}\times2\sqrt{3}$) 구조로 정육각형의 형태로 spot 이 배열되어 있으며, 또 다른 하나는 ($2\sqrt{3}\times4\sqrt{3}$) 구조로 긴 spot 이 zigzag 의 형태로 배열되어 있었다. 이러한 DMG 분자의 흡착 농도를 결정하기 위해 X-ray photoelectron spectroscopy (XPS)를 이용하였다. XPS 를 통해 알아낸 DMG 의 흡착농도는 0.33 으로 STM 관찰로 얻어진 spot coverage 0.08 과 비교하여 볼 때, STM spot 하나에 4 개의 DMG 분자가 존재한다. 따라서 DMG 는 Au(111) 표면에 분자 형태로 흡착하며, 흡착농도는 0.33 이다. 단분자층의 자기조립을 조절하면 크기와 모양이 다양한 template 가 형성되며, 이러한 2 차원 구조는 3 차원 구조체의 지지체로서 응용되므로 나노기술 응용에서 중요하다.

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The Study of Relationship between Oxygen Release and Nitric Oxide Simultaneously by Electrochemical Dual Microsensor

도현경, *이영미

*이화여대 화학나노과학 *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) and a Ag/AgCl counter/reference electrode. Working and reference/counter electrodes immersed in an optimized internal solution 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 prepared NO/O_2 dual microsensor was applied for measurements of the oxygen release from solution Human serum albumin (HSA) and powdered HSA induced by the injection of NO. In order to study the critical factors of the HSA oxygen release, the changes in the oxygen concentration induced by NO injection were also monitored for the HSA denatured by heat treatments at various temperatures. This work was supported by "GIST Systems Biology Infrastructure Establishment Grant (2010)".

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Electrochemical Properties of Alkanethiol Monolayers Adsorbed on Nanoporous Au Surfaces

추연이, 김종원

충북대 화학과

The adsorption of thiolate molecules on a flat Au surface results in the well-organized self-assemble structures through hydrophobic interactions between alkyl chains of adjacent thiolates, while the self-organization is apparently limited on curved Au nanopaticle (AuNP) surfaces. The aim of this work is to examine the characteristic electrochemical behaviors of Alkanethiol monolayers adsorbed on the curved Au surfaces compared with those on flat Au surfaces, from which the nature of thiolate monolayers adsorbed on AuNP surfaces can be elucidated. We investigate the electrochemical properties of Alkanethiol monolayers adsorbed on NPG surfaces by cyclic voltammetry and electrochemical impedance spectroscopy. The reductive desorption of alkanethiols on NPG surfaces is observed in more negative potential regions than that on flat Au surfaces due the stronger S-Au interaction on NPG surfaces. However charge-transfer resistance on the alkanethiol monolayers on NPG surfaces is smaller than that flat Au surfaces. While the electron transfer through Alkanethiol monolayers on flat Au surfaces occurs via tunneling process through the monolayer films, the redox species can permeate through the monolayers on NPG surfaces to transfer the electrons to the Au surfaces. This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation.

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Electrocatalytic reduction of hydrogen peroxide at nanoporous gold structure

박유훈, 김종원

충북대 화학과

Electrocatalytic reduction of hydrogen peroxide (H_2O_2) was investigated at nanoporous gold (NPG) surfaces. NPG surfaces were prepared by electrodeposition for Au-Ag layers on Au/Si surfaces followed by selective dissolution Ag in concentrated nitric acid. The surface structure and electrochemical area of NPG were controlled by changing the concentration ratios of $KAu(CN)_2$ over $KAg(CN)_2$ and deposition charges. The effects of different electrochemical conditions on the electrocatalysis of H_2O_2 reduction are investigated. The NPG surfaces exhibit sensitive amperometric responses for H_2O_2 reduction, from which calibration plots with higher sensitivity than a bare Au surface were obtained. This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation.

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Simple electrochemical deposition of Au nanoplates from a Au(Ⅰ) cyanide complex with unique electrocatalytic activities

서보라, 최수희, 김종원

충북대 화학과

Electrochemical deposition of Au offers a route to fabricate Au surface nanostructures. The morphology and electrochemical surface area of nanostructures can be turned by the controlling deposition conditions. Au nanoplate structures can be fabricated by a simple electrodeposition from an $Au(CN)_2^-$ without any surfactants, templates, or pre-modification of electrode surfaces. In contrast to other electrodeposited Au nanostructures, nanoplate Au structures are rich Au (110) and Au (100) crystalline domains, which exhibit unique electrocatalytic activities for oxygen reduction and glucose oxidation. An easy preparation of well-defined nanoplate Au structures will provide new opportunities as Au based substrates for other electroanalytical applications through further chemical modification of Au surfaces. This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation.

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Electrochemical Sensors for Glucose or Insulin Using Gold Nanoparticles Covered with Palladium or Ruthenium

김지영, *심준호, **이종목, ***이영미

*이화여대 나노화학과 *이화여대 신재생에너지연구센터 **이화여대 화학과 ***이화여대 자연과학대학/화학전공*

Gold nanoparticles (AuNP) coated with Pd or Ru supported on carbon were used as a nonenzymatic electrochemical sensor for detection of glucose or insulin, respectively. AuNP/Pd/C and AuNP/Ru/C electrodes were prepared by a simple spontaneous deposition of Pd or Ru onto AuNP. The modified electrodes were investigated using transmission electrode microscopy (TEM), X-ray diffraction (XRD), energy dispersive spectroscopy (EDS) to verify the morphology and to analyze the composition of respective metals. The voltammetric and amperometric measurements exhibited that the AuNP/Pd/C and AuNP/Ru/C electrodes catalyzed the oxidation of glucose and insulin at +0.25~0.3 V and at +0.6 V, respectively which are much less positive potentials when compared to previously reported researches. These results showed a considerably advanced electrocatalytic activity toward the glucose and insulin oxidation and these electrodes have potentials as promising glucose and insulin sensors. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institue of Science & Technology (DGIST), funded by MEST.

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Characterization of the Activity of Porous Metallic Electrocatalysts for Oxygen Reduction Reaction (ORR) and Study of ORR Mechanism Using Scanning Electrochemical Microscopy

양지혜, *이종목, **이영미

*이화여대 화학나노과학전공 *이화여대 화학과 **이화여대 자연과학대학/화학전공*

Pt has been known that it shows generally the best activity for sluggish oxygen reduction reaction (ORR) in polymer electrolyte membrane fuel cells (PEMFC). Research on alternative economic and efficient electrolytic materials has been performed due to the high cost and the limited supply of Pt. Therefore, we prepared a variety of porous metallic electrocatalysts by simple electrodeposition with or without controlling the microstructures called mesoporous structures. In addition to Pt (for comparison), Pd and Ir are electrodeposited on a Pt microdisk substrate. The location-dependent ORR activities of the prepared porous metallic electrocatalysts (mesoporous or not structure-controlled) are studied by scanning a small Pt-disk tip electrode using scanning electrochemical microscopy (SECM) in tip generation–substrate collection (TG-SC) mode: O_2 generated at the tip is reduced at the electrocatalyst substrate. The study of morphologies of the electrocatalysts are also obtained using SECM in TG-SC mode in a solution of reversible electroactive species ($Ru(NH_3)_6^{3+}$): $Ru(NH_3)_6^{3+}$ is reduced to $Ru(NH_3)_6^{2+}$ at the tip surface and then the produced $Ru(NH_3)_6^{2+}$ is oxidized at electrocatalyst substrate . The observed morphology and the local ORR activity of the electrocatalysts are compared and analyzed. Also, we examined the mechanism of ORR occurring at the electrocatalyst surfaces. It is already known that the ORR is 2 electron transfer reaction at Au electrode. Therefore, we prepare bare W tip and platinized Pt tip to compare with Au tip and confirm whether ORR is 2 electron or 4 electron transfer reaction using SECM in TG-SC mode This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by Ministry of Education, Science and Technology (MEST) of the Republic of Korea.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Development of an Electrochemical Glucose Sensor Based on a Micropore Working Electrode

장경, *심준호, **이영미

*이화여대 화학 나노과학과 *이화여대 신재생에너지연구센터 **이화여대 자연과학대학/화학전공*

Amperometric biosensors for glucose, a primary energy source of organisms, are important in bioanalysis. A new amperometric glucose sensor was prepared based on a micropore-type working electrode. The prepared micropore-type glucose sensor showed much improved sensitivity due to the three-dimensional geometric structure in comparison with a conventional sensor based on a planar-type disk working electrode. Also, this sensor was able to possess sufficient selectivity for glucose over general biological interferents by further modification with silanizing exterior surface of glass sheath and electrochemical deposition of Pt. The optimized working electrode potential was +0.35 V (vs. S.C.E.) for electrochemically measuring glucose. The glucose sensors are expected to be applied to biological research. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by Ministry of Education, Science and Technology (MEST) of the Republic of Korea.

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Effect of proton availability and hydrogen bonding in electrochemistry of quinines in aqueous solutions

홍희정, 박원철, *김성현

*건국대 생명공학과 *건국대 특성화학부생명공학과*

We have synthesized quinone molecules that have long alkyl side chains of different lengths (n = 4, 8, 10, 16) and alkyl spacers with a -SH group. These molecules were self-assembled on Au electrodes and their electrochemical properties have been studied using cyclic voltammetry. As the chain length increases, a single redox pair begins to split to two redox pairs in which the new pair is very irreversible and grows at the expense of the main redox peak when a full monolayer is formed. This was interpreted in terms of poor proton availability through the long alkyl chain. Upon formation of a mixed monolayer with a simple alkanethiol whose length is the same as that of the spacer, two redox pairs become a single pair, indicating rapid proton access to the quinone group. Even at the full monolayer, two redox pairs also become a single pair when the intramolecular hydrogen bonding was blocked by attaching an actyl group to the amine site in the alkyl chain.

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A microbial fuel cell using a polyviologen-modified anode

김준현, 박원철, *김성현

*건국대 생명공학과 *건국대 특성화학부생명공학과*

In a traditional microbial fuel cell (MFC), dissolved viologen has been used as a mediator because it transfers electrons from microbes to anode. Problems are, however, that electron-transfer rate depends on the diffusion rate of viologen molecules, which put a serious limitation on the performance enhancement. The best way should be to form a molecular wire connecting the microbe and the electrode. Here we synthesized polyviologen (PV) as a possible molecular wire and studied its electrochemical behavior on the electrode surface under various conditions. When applied to the MFC anode, the cell potential was rapidly stabilized, indicating the positive effect of this molecule.

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Effects of carbon nanotube layer on the electrocatalytic reduction of O2 at a "wired"-BOD cathode

강찬, 송지선, 신효설

전북대 화학과

Effects of carbon nanotube (CNT) layer for immobilizing enzyme bioelectrocatalyst on the catalytic activity were investigated. A cathode with bilirubin oxidase (BOD) wired by the redox polymer PAA-PVI-[Os(dcl-bpy)2Cl]+/2+ over a single-walled carbon nanotube (SWNT) electrode on a glassy carbon surface was prepared. Electron transfer rate in the carbon nanotube layer and the redox hydrogel film was compared. The CNT layer provides a good contact with the enzyme-redox polymer film and a rough surface with large microscopic surface area giving high density of enzyme molecules with thinner redox hydrogel film. An enhancement of current density by about 50% with the BOD cathode on the CNT-modified electrode in comparison to that on a bare GC surface was measured. Systematic studies with different coverage of CNTs, BOD wt %, and catalyst amount were carried out.

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Selective adsorption of dithiolate-modified multi-wall carbon nanotubes onto alkanethiol self-assembled monolayers on Au(111)

김혜령, 정창훈, 김잔디, *김세철, *김혜란, *김영래, 이충균

*충남대 화학과 *충남대 분석과학기술대학원*

3 차원 나노구조체 형성을 위해서 Au(111) 표면에 알킬체인 길이가 서로 다른 4 가지 alkanethiol SAMs 를 형성한 후에 dithiolate MWCNT 를 접근시켜 AFM 으로 MWCNT 의 결합여부를 관찰하였다. 1,3-propanedithiol 로 변화시킨 MWCNT 를 thiol SAMs 에 도입해 보았을 때는 길이가 짧은 3C thiol SAMs 에는 결합하지만 긴 체인인 12C thiol SAMs 에서는 결합하지 않는 것을 관찰하였다. 하지만 1,16-hexadecanedithiolate MWCNT 는 12C thiol SAMs 에 결합하였다. 이를 통해서 thiol SAMs 알킬체인 길이와 dithiolate MWCNT 의 알킬체인 길이 간의 경쟁으로 MWCNT 가 SAMs 기질에 선택적으로 결합함을 알 수 있었다. 패턴화된 MWCNT 표면을 만들기 위해서 PDMS 를 이용해서 3C thiol 과 12C thiol 로 각각 표면을 형성한 후에 1,6-dithiolate MWCNT 를 결합시킴으로써 3C thiol 에만 MWCNT 가 결합하는 것을 관찰할 수 있었다. 이를 응용하여 MWCNT 를 패턴화하는 기술로 발전시킬 수 있을 것이다.

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Simultaneous electrochemical detection of ascorbic acid, dopamine, and uric acid on a graphite electrode

강찬, 신은정, 신효설

전북대 화학과

Ascorbic acid (AA), dopamine (DA) and uric acid (UA) are compounds of interest because of their biological importance and their electrochemical simultaneous determination on an edge plane graphite (EPG) electrode was studied. It is generally not easy to separate each individual oxidation wave at conventional electrodes with their close oxidation potentials. In this study, an EPG electrode, whose surface was simply roughened, was employed and three well separated individual waves were observed. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used to obtain the calibration curves. For each component, detection limit, sensitivity, and dynamic concentration range was determined. Any component of in their mixture of AA, DA and UA was also analyzed while concentrations of the other two species are fixed constant.

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Formic Acid Catalytic Properties of Electrochemically deposited Palladium Nanoparticles on Indium Tin Oxide Electrodes

김병권, 서대하, 송현준, 곽주현

KAIST 화학과

Palladium nanoparticles were electrochemically deposited on indium tin oxide electrodes by cyclic voltammetric method and their nanoparticle size was demonstrated by scanning electron microscopy. The electrochemical deposition conditions of the palladium nanoparticles were varied according to a scan rate of 1 mV/s, 5 mV/s, and 10 mV/s. As the scan rate was decreased, the size of the palladium nanoparticles increased, but the formic acid catalytic property was weakened. With regard to cycle number, with increased cycling, the size of the palladium nanoparticles increased but the formic acid catalytic property decreased. Despite the increase in particle size, the current density of formic acid oxidation decreased due to a reduction of the catalytic activity of the palladium nanoparticles. In our experiments, the best results were obtained with a scan rate of 10 mV/s scan rate and 1 cycle deposition.

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Direct observation of Cu UPD and OPD process on Au(111) surface using in-situ STM and AFM

Acdac Rashida

충남대 화학과

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대한화학회 THE KOREAN CHEMICAL SOCIETY

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A glucose biosensor based on the enzymatically precipitated prussian blue onto the synthesized gold-coated magnetic microparticles

정혜영, 박준희, 곽주현

KAIST 화학과

The gold-coated magnetic microparticles (gold-coated MMPs) were synthesized by commercially available polystyrene spheres as the core and by the gold nanoparticles adsorbed on the thiol-modified polystyrene spheres as seeds. A subsequent reducing process of gold ions made outer gold layer and in-depth characterization of the gold shell formation was studied with scanning electron microscopy, energy-dispersive X-ray spectroscopy, cyclic voltammetry. The gold-coated MMPs were exploited for an electrochemical glucose sensing. Gold shell outside magnetic polystyrene beads can provide both the enhanced conductivity between particles for electrochemistry, the sulfur-gold chemistry for the surface modification, and the seeds for the precipitation of prussian blue. Combining these advantages, glucose oxidase was covalently immobilized on the gold-coated MMPs for the enzymatic precipitation of prussian blue on the surface of particles in the colloidal solution. By applying the external magnetic field, electrical contact of each particle to the electrode surface generated the electrochemical signal depending on the concentration of glucose. These results demonstrated that the gold layer serves as the seed layer for prussian blue keeping good enzymatic activity and the enhanced electrical conductivity. This unprecedented approach successfully proposed the applicability of the magnetic core-gold shell structures to the electrochemical biosensor.

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Electrochemical property and structural investigation of anion substituted cathode materials for Li-ion rechargeable battery

신병철, 이경은, 이영일

울산대 화학과

Fluorine substitution at the oxygen site of the cathode active materials like $LiFePO_4$ for lithium ion batteries attracts much attention in recent years. There has been considerable interest in $LiFePO_4$ as a cathode active material in Li-ion cells because of its superior cost, safety, stability and low toxicity. The major drawback has been the low electronic conductivity achievable at even moderate synthesis. Optimized $LiFePO_4$ cathode provides a reversible capacity of 150~160 mAh/g with a very flat charge/discharge potential of 3.4 V versus Li/Li^+ at current of $0.1mA/cm^2$. Compared to the presently used other anion substitution result, the $LiFePO_4$ has intrinsically lower energy density, in addition to its natural drawbacks such as low electronic and ionic conductivities. Numerous studies have devoted to understand the relationship between the structure and the ionic and electronic transport properties and how these properties can be improved. For overcoming this problem, many studies have been found such as anion substitution, especially fluorine substituted $LiFePO_4$ was reduce main unit cell volume by induced binding energy. The crystal structure of these materials was stabilized by partially substituting fluorine for oxygen site. The electronic and local geometric structural characterization for $LiFePO_4/F$ was supposed to using in situ XAFS and ^7Li MAS NMR. In situ X-ray absorption study has been performed to understand of structural change of $LiFePO_4/F$ composite during the discharge process. The electrochemical measurements, XRD, and SEM with EDS were also performed.

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Synthesis of Iron-hippuric acid Complex and its application to electrochemical amperometric immunoassay for hippuric acid

최영봉, 김혁한

단국대 화학과

The electrochemical immunoassay system needs to label antigen or antibody with electro-active materials such as metal complex and metal nanoparticles. The series of novel, electro-active antigen-HA-Iron(II/III) complex was prepared and then characterized using electrochemical techniques. The newly synthesized antigen-HA-Iron(II/III) complex presented here are described in shorthand as [Fe(CN)5(aminomethylpyridine-hippuric acid)]2/3-, was detected on the carbon nano-tube paste electrodes. The carbon nano-tube paste electrodes compose of the multi-wall carbon nano-tube and carbon ink. Surface of the carbon nano-tube paste electrodes were identified by SEM image. The electrochemical immunoassay comprised antibody-HA and then applied antigen-HA-Fe in the micro-tube. The electrical signals were measured by voltammetry technique. Because of its diffusion effect of heavy molecule, the Electrochemical immunoassay is a homogeneous competitive immunoassay method based on the decrease in electrical signal of Iron-labeled small antigens(HA) when bound by specific antibody. 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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Synthesis and electrochemical characteristics of Osmium redox hydrogel containing hyppuric acid and Its application of immunoassay

이예림, 김혁한, 최영봉

단국대 화학과

Urinary hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring of exposure to toluene is very important in occupational health care. We propose a hydrogel-based electrochemical immunoassay for rapid and quantitative detection of HA. The system employs a conjugate of Osmium [Os(bpy)2] and hippuric acid (HA) and then Os(bpy)2-HA reacts with poly(vinyl imidazole) (PVI), a hydrogel polymer. The competition between hippuric acid (HA) and PVI-Osmium-HA generated electric signals proportional to HA concentration. The electrochemical immunoassay was comprised with immobilization of PVI-Osmium-HA on the screen printed carbon electrode (SPCEs) and then apply the mixture antigen (HA) and HA-antibody. The electrical signal was measured by voltammetry technique. The resulting currents were linearly related with the concentration of HA complex. Also the structures of Osmium compounds have been identified by the spectroscopic method and the electrochemical method.

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Straightforward fabrication of amperometric glucose microsensors for long-term use in physiological milieu: Use of amine-modified*exp* hybrid xerogel matrixes

김영국, 허민, 차근식, 남학현, 신재호

광운대 화학과

Glucose biosensors have been developed further more. The exact measurement of glucose concentration is important because glucose concentration in blood is the yardstone of diabetes mellitus patient whether or not. Generally speaking, spectroscopic and electrochemical methods are famous for conventional glucose measuring methods. Those methods have some obstacles, such as the short biosensors lifetime, sophisticated fabrication methods and inaccuracy blood glucose concentration due to the interference effect. To eliminate interference effect, simplify fabrication steps and lengthen biosensors lifetime, I choose the introduction of a various of sol-gel process. To optimize the glucose biosensor, sensor membrane composition is changed and researched the influence of biosensors characteristics. We investigated accordance between a standard equipment and optimized biosensors on from real blood sample to sample with interference agents.

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Amperometric sensing of *S*-nitrosothiols based on their photo-induced decomposition: Optically switchable determination of nitric oxide and *S*-nitrosothiols

성다연, 홍성아, *차근식, *남학현, *신재호

*광운대 화학 *광운대 화학과*

S-Nitrosothiols (RSNOs), a group of potential nitric oxide (NO) storage, transfer, and delivery vehicles regulate several biological processes, including vasodilation, platelet activation, neurotransmission, and tissue inflammation. Small-molecule RSNOs such as *S*-nitroso-*N*-acetyl-*DL*-penicillamine (SNAP), *S*-nitroso-*N*-acetyl-*L*-cysteine(SNAC), and *S*-nitrosoglutathione (GSNO) have been extensively investigated as conveyance for NO with well-documented antimicrobial and antithrombotic effects. Various analytical methods have been developed for determination of physiological levels of RSNOs. Several reported sensors have previously utilized catalyst (e.g., copper(II) and organoselenium) to generate NO by decomposing RSNOs that are either endogenously present in biological systems or have been incorporated into monolayers or hydrogels. However, previous sensors have a difficulty in distinguishing NO signal from RSNO signal. Herein, we report on a new approach to design an electrochemical sensor for a simple, photolytic detection of SNAP as a small-molecule RSNO. The sensor can distinguish signals that NO and photo-decomposed NO from the RSNO. Using of an optical fiber in the sensor makes easy to miniaturization and good portability. In a further study, the use of optical fibers will allow the sensor to apply an *in vivo* milieu. The fabrication process of the optical fiber sensor is easy and simple. Carbon paste is screen-printed on the optical fiber surface. The carbon surface is then platinized in a 3% chloroplatinic acid solution with cyclic voltammetry. The sensor's optimization saccording to the optical property of RSNO, and each signal depending on the various compounds (e.g.,SNAP, GSNO and SNAC) will be discussed. In addition, this system will apply to human blood serum.

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All-solid-state ion-selective membrane electrodes based on use of conducting polymers: High stability and reliability for long-term use

허민, 정연준, *진선민, 이재선, 김인태, 차근식, 남학현, 신재호

*광운대 화학과 *광운대 화학과*

Potentiometric ion-selective membrane electrodes (ISMEs) have been extensively used for ion analysis in clinical, environmental, and industrial fields, owing to its wide response range (4 to 7 orders of magnitude), no effect of sample turbidity, fast response time, and ease of miniaturization. Poly(vinyl chloride) (PVC) has been widely employed to fabricate solvent-polymeric ISMs due to its excellent electrochemical properties. However, PVC-based ISMEs have some drawbacks including low thermal durability, low mechanical strength, and poor adhesion toward electrode surfaces. Thus, its utility to all-solid-state electrodes has been restricted. Considerable attention has been given to alternative use of room-temperature vulcanizing (RTV)-type silicone rubber (SR) owing to its strong adhesion and high thermal durability. Unfortunately, the high membrane resistance of SR-based ISMs (2 to 3 higher orders of magnitude compared to those of PVC ones) has significantly restrict its application. Herein we demonstrate a new method to reduce membrane resistance via addition of conducting polymers [i.e., (poly (2,6-didodecyl-4-ethynyl-8-(2,5-bis-nonyloxy-phenylethynyl)-benzo[1,2-d;45-d']bisthiazol and poly (2-(2,3-dihydrothieno[3,4-b][1,4]dioxin-7-yl)-9-nonylcarbazole))] into the SR-based ISMs.

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Planar-type all-solid-state sensors for potentiometric measurements of polyanionic humic acid in soil samples

구현우, 강영재, 이재선, *임우진, *신국식, *이상은, 차근식, 남학현, 신재호

*광운대 화학과 *한경대 기후변화연구센터*

Humic acid, a part of naturally synthesized organic substances in soil is known to improve soil fertility. The conventional techniques for measuring soil humic acid are mostly based on the determination of total organic carbon (TOC) contents. However, their utility in soil analysis has been limited due to several drawbacks, including complicated sample pre-treatment, expensive instrumentation, and time-consuming process. To overcome such shortcomings, an electrochemical method may provide a promising alternative. Indeed, the high-charge density polyanionic structure of humic acid in a basic solution allows for its potentiometric measurement. Notably, the concentration of clinically important polyions such as heparin, protamine, and oversulfated chondroitin sulfate (OSCS) has been successfully determined by measuring nonequilibrium boundary potential at the polymeric membrane/sample interface. Herein we demonstrate a robust sensing tool for the determination of humic acid in soil samples via use of both all-solid-state sensor technique and flow-injection analysis. To eliminate interferences from nitrate and chloride, the composition (e.g., type, pH, and concentration) of a sample extraction solution is optimized. Furthermore, the levels of humic acid in soil samples determined using the potentiometric all-solid-state sensors are compared to the values obtained by the conventional TOC analysis.

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Homogeneous Deposition of Platinum Nanoparticles onThe hollow core–mesoporous shell carbon for Proton Exchange Membrane Fuel Cell

송민영, *김민식, *김정호, **Nitin Chaudhari, kiran chaudhari,** 김민우, 임신묵, **양대수, * 유종성

*고려대 소재화학과 *고려대 신소재화학과 **고려대 신소재화학*

The hollow core–mesoporous shell (HCMS) carbon has unique structural characteristics such as large specific surface area and mesoporous volume, ensuring uniform dispersion of the supported high loading (60 wt%) Pt nanoparticles with small particle size, and well-developed three-dimensionally interconnected hierarchical porosity network, which are highly desired for a cathode catalyst support in low temperature fuel cells.A simple and efficient approach has been developed for synthesis of carbon-supported Ptnanoparticles (NPs) that combines homogeneous deposition (HD) of Pt complex species through a gradualincrease of pH realized by in situ hydrolysis of urea and subsequent uniform reduction by ethylene glycol(EG) in a polyol process, giving control over the size and dispersion of Pt NPs. With increasing amount of urea in the starting Pt salt aqueous solution, the size of Pt complex species decreases and so does that of the metallic Pt NPs. The excellent electrocatalysis ability of the Pt catalysts produced by HD-EG is demonstrated through the determination of electrochemical surface area and fuel-cell polarization performance. The Pt NPs deposited on hollow core–mesoporous shell (HCMS) carbon by the HD-EG strategy show smaller size with more uniform dispersion, higher Pt utilization efficiency, and considerably improved fuel-cell polarization performance compared with the Pt NPs prepared by conventional sodium borohydride reduction approach. The HCMSC-supported Pt(60 wt%) cathode catalyst has demonstrated markedly enhanced catalytic activity toward oxygen reduction and greatly improved PEMFC polarization performance compared with carbon black Vulcan XC-72 (VC) supported ones.

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Bioengineered recombinant single-chain fragment variable (scFv) antibody for electrochemical immunoassay of B-type natriuretic peptide (BNP)

최정연, *맹보희, 이지연, 김석규, *김용환, 차근식, 남학현, 신재호

*광운대 화학과 *광운대 화학공학과*

Immunosensors are used to detect or quantify disease substances known as biomarkers in clinical diagnosis. In immunosensor applications, it is important that antibodies are immobilized on the immunosensor surface. Typically, the immobilization of antibody fragments is conventionally achieved using physical adsorption or covalent cross-linking methods. In these methods, however, antigen-binding activity can be lost and binding sites on the antibody can be randomly coupled with several reactive moieties on the sensor substrate surface. Thus, there is an increasing need for a technique of achieving well-oriented immobilization of antibody fragments in a small area without decreasing their binding affinity for target molecules, especially for miniaturized diagnostic devices. Herein, we demonstrate an electrochemical BNP immunosensor by employing a recombinant single chain fragment variable (scFv) antibody for a highly sensitive detection of B-type natriuretic peptide (BNP) as a model target protein. BNP is one of the most important biomarker in early diagnosis of congestive heart failure. The recombinant scFv consists of the antibody variable heavy and light pairs. Recombinant scFv antibodies (28 KDa) contain no antibody constant regions, typical of traditional antibodies, and represent the smallest functional domains of an antibody necessary for the high-affinity binding to antigen. ScFvs have metal-binding amino acids (i.e., histidine) in the scFv peptide linker. The binding of hexahistidine (His6) sequence tags to Ni2+chelates of nitrilotriacetic acid (NTA) has been widely known as a powerful affinity. Using this system, it can be immobilized onto a gold surface in a favorable antigen-binding orientation at high density that significantly increased assay sensitivity.

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Nonenzymatic Amperometric Glucose Sensor Based on Three-Dimensional Nanoporous Ruthenium Oxide Framework

강민경, *심준호, **이영미, ***이종목

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In the present study, a nonenzymatic amperometric glucose sensor has been attempted based on the three-dimensional nanoporous ruthenium oxide for the enhancement of sensitivity. For comparison purpose, the electrodeposition process of Ru on a gold substrate electrode was conducted by potentiostatic or cyclic voltammetric method and in the presence or absence of a nonionic surfactant. The surface morphology and thickness of the prepared nanoporous ruthenium oxide framework was characterized using scanning electron microscopy and transmission electron microscopy. Chronoamperometry was used to evaluate glucose detection and selectivity against L-ascorbic acid or 4-acetamidophenol. Nanoporous Ru electrode shows significant effects on increasing glucose oxidation signal compared with bare Au or Pt electrode presumably due to surface area increase by nanostructure.

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Enzyme Encapsulation in conducting polymer fiber structures for amperometric Glucose Biosensor

정신환, *이영관, 손용근

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A bundle of microfiber/tubule structures comprised of conducting polymer was fabricated onto an ITO electrode to enhance current collection efficiency in a biosensor system. A glucose biosensor adopting the bundle system was manufactured by capturing enzyme of glucose oxidase covered with a thin Nafion film. Chronoamperometric current response from the oxidation of the hydrogenperoxide was measured. The glucose substrate was allowed to pass through the Nafion membrane from the bulk test solution to the enzyme. The enzyme can produce hydrogenperoxide and its oxidation current was measured with a constant potential. This sensor provided a current response linearly dependent on the concentration of the substrate. The manufacturing procedure was stuied with SEM methode.

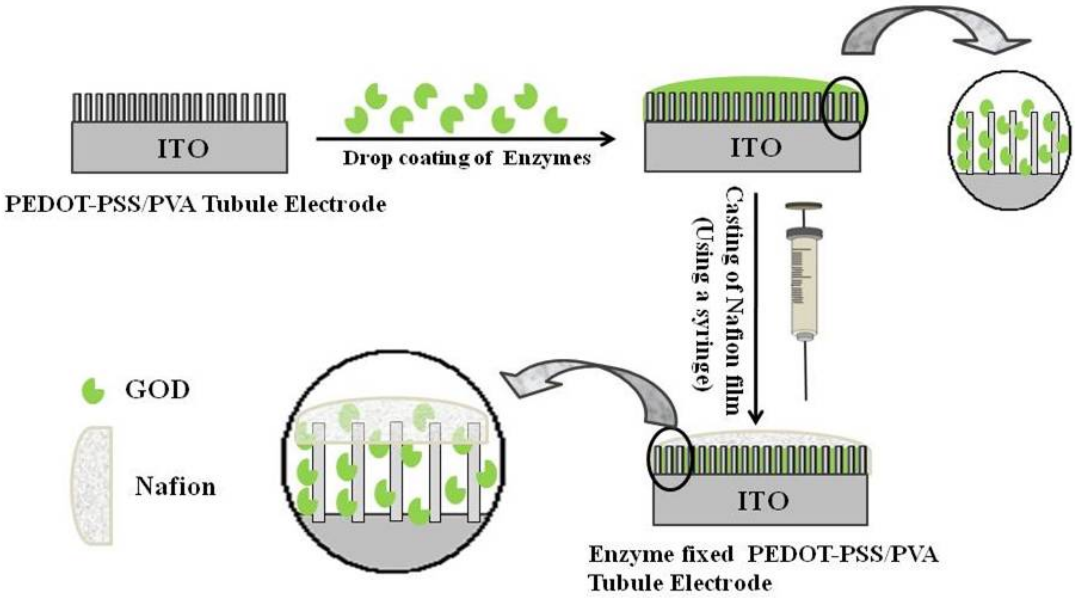

Fig. 1. Schematic diagram of the enzyme immobilized conducting polymer fiber structures.

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Formation of self-assembled 3-mercaptopropionic acid monolayer on the gold nanoparticle-modified indium tin oxide (ITO) glass: Application to the electrochemical detection of Cu^{2+} ion

이충구, 이승현, *이영관, 손용근

*성균관대 화학과 *성균관대 화학공학과*

We have studied an electrochemical sensor for the detection of copper ion by using a 3-mercaptopropionic acid (3-MPA) formed on gold nanoparticle-modified indium tin oxide (ITO) glass. First, gold nanoparticle-modified ITO glass (AU-NPs/ITO) were prepared through direct electrochemical deposition from 1 M H_2SO_4 containing 1 mM $HAuCl_4$. Self-assembled monolayer (SAM) of 3-MPA was formed at gold nanoparticle surfaces using a 1 mM solution of the modifier in de-ionized water (D.I water). The Au-NPs/ITO electrode surfaces were characterized by UV-vis, field emission gun scanning electron microscopy (FESEM) and cyclic voltammetry using a 0.05M H_2SO_4 solution. 3-MPA/Au-NPs/ITO electrode surfaces was characterized by FT-IR and FESEM. Finally the modified electrode was used for the electrochemical analysis of trace amount of copper ion by square wave anodic stripping voltammetry (SWASV) method.

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One-step synthesis of silver nanoparticles for printed electronics: metallization behavior at low temperature

이승현, 손용근

성균관대 화학과

In order to form a conducting network at low temperature in printed electronic circuits, ink-jet printable inks are asked to possess small particle size because the melting point of nanoparticles has been inversely correlated with their radius. Therefore we prepared smaller silver nanoparticles than issued ones by using one-step synthesis through direct ligand exchange. Wet chemical reduction was performed under the conditions of high concentration and bulk scale (above 1L). TEM image showed that nanosized spherical particles with 5.4±0.7nm were obtained. The metallization behavior of the silver nanoparticles was observed by SEM method. The grain boundary appeared at low temperature (below 200℃). The products were characterized by using UV/Vis, FT-IR, NMR, TEM, SEM, XRD, TGA and DSC. Silver colloidal inks made from these particles were stable for a long time.

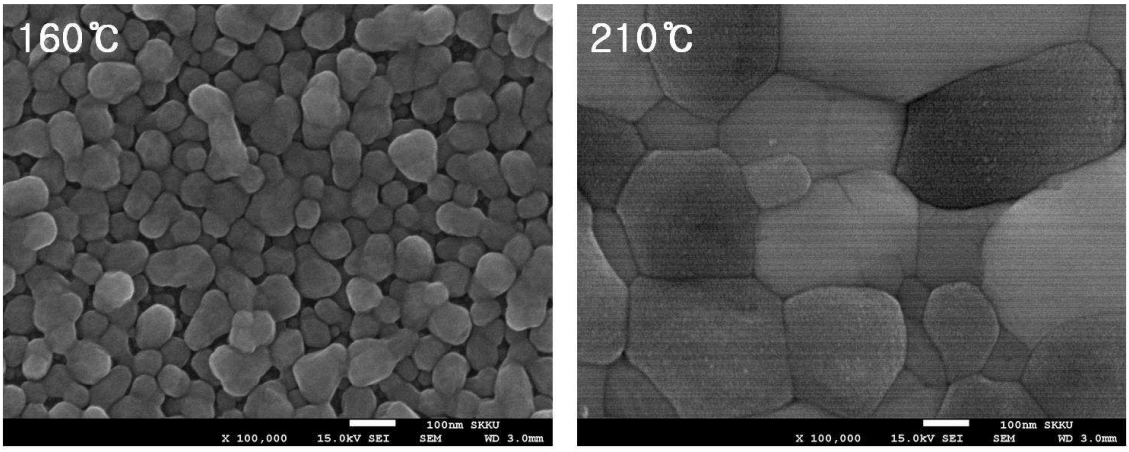

Figure 1. SEM image of silver nanoparticles annealed at 160 and 210℃ for 30 min.

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Facile synthesis of multimodal porous carbons with tunable open and close mesopore morphology as a cathode catalyst support in proton exchange membrane fuel cell

임신묵, *김민식, *김정호, **kiran chaudhari, Nitin Chaudhari, *Paul Gouri Sankar,** 김민우, 송민영, **양대수, 김윤경, *유종성

*고려대 소재화학과 *고려대 신소재화학과 **고려대 신소재화학*

Three-dimensional mesoprous materials have attracted much attention in the last decade due to their wide range of applications ranging from catalyst support till hydrogen storage. A simple approach has been to develop mesoporous carbon with controlled open & close mesopore architecture. The multimodal carbon with open pore was carbonized after removing PS spheres to develop open pore and multimodal close pore carbon was formed where PS spheres were allowed to remain as they are. The PS spheres act as carbon precursors that cover silica in the multimodal close porous carbon. Facile synthesis of multimodal porous carbons with tunable open and close mesopore morphology as a cathode catalyst support in proton exchange membrane fuel cell are presented.

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Erythrocyte-like hollow carbon capsules and their application in proton exchange membrane fuel cell

김정호, 김민식, *Nitin Chaudhari, *kiran chaudhari, Paul Gouri Sankar, *김민우, *임신묵, **양대수, *송민영, *김윤경, 유종성

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Hierarchical nanostructured erythrocyte-like hollow carbon (EHC) with a hollow hemispherical macroporous core of ca. 230 nm in diameter and 30 - 40 nm thick mesoporous shell was synthesized and explored as a cathode catalyst support in proton exchange membrane fuel cell (PEMFC). The morphology control of EHC was successfully achieved using solid core/mosoporous shell (SCMS) silica template and different styrene/furfuryl alcohol mixture compositions by nanocasting method. The EHC-supported Pt (20 wt%) cathodes were prepared and have demonstrated markedly enhanced catalytic activity towards oxygen reduction reaction (ORR) and greatly improved PEMFC polarization performance compared to carbon black Vulcan XC-72 (VC)-supported ones probably due to superb structural characteristics of the EHC such as uniform size, well-developed porosity and large specific surface-area and pore volume. In particular, Pt/EHC cathodes exhibited ca. 30 - 60% higher ORR activity than commercial Johnson Matthey Pt catalyst one at a low catalyst loading of 0.2 mg Pt cm-2 on the cathode

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Ion exchange adsorption property of carbon nanotubes on a glassy carbon electrode

강찬, 신효설, 송지선, 신은정

전북대 화학과

The cation-exchange property of oxidatively treated carbon nanotubes (CNTs) was studied. Single-wall carbon nanotubes (SWNTs), which were oxidatively treated, were immobilized on a glassy carbon surface and, on this CNT-modified electrode, Cu(II) ions were spontaneously adsorbed and their redox waves were electrochemically measured. It is suggested that the adsorption of the cationic Cu(II) ions occurs by their electrostatic interaction with the negatively charged carboxylic anions on the CNTs after the ion-exchange with protons. The surface coverage of the adsorbed Cu(II) ions depending on the dipping time, the amount of immobilized CNTs, and the Cu(II) concentration was estimated from the electrochemical chronocoulometric measurements.

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Effect of pH on Electrocatalytic Properties of Supported Pd Catalysts in Proton Exchange Membrane Fuel Cell

김민식, 김정호, *Nitin Chaudhari, *kiran chaudhari, *김민우, *임신묵, *송민영, **양대수, 유종성

*고려대 신소재화학과 *고려대 소재화학과 **고려대 신소재화학*

In this study, urea-assisted homogeneous deposition (HD) strategy was employed to synthesize Vulcan XC-72 (VC)-supported Pd (60 wt%) catalysts under various initial pH conditions. In-situ gradual generation of hydroxide ions through hydrolysis of urea at elevated temperature results in HD of Pd species on the VC support. In addition, it was found that the initial pH value of the staring solution has significant influence on the Pd metal particle size and the catalytic activity of the supported Pd catalyst. Under most pH values investigated (i.e., higher than 5~6), the VC-supported Pd catalysts prepared by the HD approach have shown smaller metal particle size with better particle dispersion. As prepared catalyst demonstrated greatly improved anode catalyst performance over the one prepared by well known impregnation-NaBH4 reduction at pH 7~8 in proton exchange membrane fuel cell. The results presented in this study highlights that highly efficient Pt-based catalysts can be prepared by the HD strategy through the control of the initial pH value in the starting solution.

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Hollow Core-Mesoporous Shell Carbon Sphere for High Li Storage Capacity and Better Cycling Performance

김민식, 김정호, *Nitin Chaudhari, *kiran chaudhari, *김민우, *임신묵, **양대수, *송민영, 유종성

*고려대 신소재화학과 *고려대 소재화학과 **고려대 신소재화학*

Hollow Core-Mesoporous Shell Carbon sphere (HCMSC) with hierarchical nanostructure was prepared and explored as anode in Li ion battery. Compared with commercial graphite, ordered mesoporous carbon (CMK-3), the HCMSC not only demonstrates higher Li storage capacity, but also better cycling performance and rate capability. HCMSC possesses unique structural characteristics such as large surface area and mesopore volume, particularly the multimodal porositiy composed of well-developed 3D interconnected mesopores embedded in the mesopore shells, facilitating fast mass transport and charge transfer. The enhancement in anode performance especially in the cycling performance and rate capability is mainly attributable to the superb structural characteristics of the HCMSC particularly the macropore of core encapulated in well-developed 3D interconnected mesoporous shell, which act as efficient Li storage and buffer reservoirs to reduce volume change during the charge–discharge cycling especially at high rates.

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Effect of MnO_2nanoparticle integration into the multilayered graphene oxide nanosheets for supercapacitors

이태민, *김병수

*울산과학기술대 나노생명화학공학부 *울산과학기술대 친환경에너지공학부*

As a complementary system between capacitors and batteries, supercapacitors have attracted a great deal of attention due to its faster power delivery and higher power densities than batteries. Various materials have been investigated as the electrode for supercapacitors, including carboneous materials, conducting polymers, and transition-metal oxides. In particular, the graphene oxide(GO), one of the most widely used derivatives of graphene, has a large surface area with a controllable surface necessary for this application based on a flat carbon form. Manganese oxide (MnO_2) is generally considered to be the most promising transition metal oxide for supercapacitors because of its high-energy density, low cost, environmental friendliness, and natural abundance. In this study, we demonstrate integration of MnO_2 into the multilayered thin films of graphene oxide nanosheets assembled by layer-by-layer (LbL) methods as a means to improve the electrochemical properties for supercapacitor application. We expect that the assembled GO/MnO_2 nanocomposite thin film electrodes exhibits a long period stability with an excellent electrochemical performance compared to GO/GO multilayered films without nanoparticles. We further demonstrate the hybrid nanocomposite films of GO/MnO_2 is very promising material for the next generation flexible electrode and high performance electrochemical supercapacitors.

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A study for the improvement of switching speed of an electrochromic cell

오지혜, 박후근, 도영락

국민대 생명나노화학과

We studied an electrochormic cell containing biphenyl dicarboxylic acid diethyl ester (DEB), which showed a reversible color change between transparent and yellow under an applied voltage of less than 3.5V by an electrochemical reaction. To improve the switching speed of the electrochromic cell, we changed many factors such as cell thickness, area, and applied voltage. N-methyl pyrrolidione (NMP) was used as a solvent after removing water by a molecular sieve. A tetra-n-butylammonium perchlorate (TBAP) electrolyte solution containing DEB as a yellow dye and ferrocene as a counter redox species was sandwiched between ITO-coated glass substrates using Surlyn tape.

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Electrochemical preparation of Indium sulfide thin film as a buffer layer of CIGS solar cell

김현진, 김규원

인천대 화학과

Recently, numerous studies for Solar cells based on Cu(In,Ga)Se2 (CIGS) have been reported. Especially CdS has been used for buffer layer which is placed between absorber layer and window layer. Toxic and expensive CdS buffer layer can be replaced by non toxic and relatively cheap In2S3. In2S3 buffer layer is normally produced by using evaporation technique. In this study, we report electrochemical method for producing In2S3 layer onto Indium tin oxide (ITO), which is cheaper and faster than evaporation technique. It is also demonstrated that the band gap of In2S3 is changed with temperature and can be optimized.

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Formic Acid Oxidation on Bi-modified Pt Nanoparticles of Various Sizes

김영래, *정창훈, *김잔디, 김세철, *김혜령, 김혜란, *이충균

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This work presents oxidation of formic acid on Bi-modified Pt nanoparticles of various sizes. The sizes of the studied Pt nanoparticles range from 1.5 to 5.6 nm (detailed in Rhee, C. K.; Kim, B.-J.; Ham, C.; Kim, Y.-J.; Song, K.; Kwon, K. Langmuir 2009, 25, 7140-7147), and the surfaces of the Pt nanoparticles are modified with irreversibly adsorbed Bi. The investigated coverages of Bi on the Pt nanoparticles are 0.12 and 0.25 as determined by coulometry of the oxidation of adsorbed hydrogen and Bi, and X-ray photoelectron spectroscopy. The cyclic voltammetric behavior of formic acid oxidation reveals that the adsorbed Bi enhances the catalytic activity of Pt nanoparticles by impeding a poison-forming dehydration path with a concomitant promotion of a dehydrogenation path. The chronoamperometric results indicate that elemental Bi and partially oxidized Bi are responsible for the catalytic enhancement, when the Bi coverages on Pt nanoparticles are 0.12 and 0.25, respectively. The size effect of Bi-modified Pt nanoparticles in formic acid oxidation is discussed in terms of specific activity (current per unit surface area) and mass activity (current per unit mass).

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The Electrochemical STM work about CO preoxidation on a modified Pt(111) surface with Ru

김세철, *김잔디, *정창훈, *김혜령, 김영래, 김혜란, *이충균

*충남대 분석과학기술대학원 *충남대 화학과*

Electrochemical scanning tunneling microscopy was used to study the structural evolution of adsorbed CO during preoxidation on Pt(111) modified with spontaneously deposited Ru. During the preoxidation process, a phase transition was observed from (2´2)-3CO-a to (√19´√19)R23.4°-13CO via the transient structures (2´2)-3CO-b and (1´1)-CO. A comparison of these structural changes with those that occur on unmodified Pt(111) revealed that the presence of Ru resulted in higher populations of transient structures at lower potentials and a cathodic shift in the potential at which preoxidation is complete. These observations are discussed in terms of increased mobility of adsorbed CO in the presence of Ru.

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Crystalline Size-Control of $LiMn_2O_4$ for Cathode of Li-ion Batteries

김주성, *여인형, **조원일, ***엄광섭, ****모선일

*아주대 화학과 *동국대 화학과 **KIST 에너지환경연구부 ***아주대 NT.IT Fusion Tech ****아주대 에너지시스템학부*

Spinel $LiMn_2O_4$ becomes one of the most promising candidates for rechargeable Li-ion batteries due to its intrinsic advantages: structural stability with insertion/desertion, high voltage, low cost, and environment. In addition, morphology, including crystalline size, plays a critical role in electrochemical activities for improved battery performance, since it greatly effects the surface area-to-volume rate and Li-ion diffusion length. In this study, the controling of crystalline size and morphology of spinel $LiMn_2O_4$ was accomplished by synthesizing amorphous nano-sized MnO_2 through the reactions of Mn^{2+} and Mn^{7+} in the aqueous solution. Nano-sized MnO_2 was refluxed in the acetonitrile solution containing LiI, then annealed at varying temperatures within 700 ~ 850℃ to achieve high crystallinity and to control the size ranged from 200 ㎚ to 2 ㎛. The crystal structure and the size of these materials were investigated by x-ray diffraction and electron microscopic methods. Size and morphology effects of these different $LiMn_2O_4$ as cathode material are presented and compared based on the battery performances and their electrochemical reactions.

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Influence of Particles Size and Crystallinity of LiV_3O_8 on the Battery Performance of LiV_3O_8/PPy composite film

Quang-thao Ta, *엄광섭, **여인형, ***조원일, 모선일

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The lithium trivanadate (LiV_3O_8) is interesting as a candidate material for lithium rechargeable batteries with potential capability to provide high capacity and good cycle stability. However, it has low electrical conductivity, which is a critical disadvantage as battery electrode material. In this work, to improve the conductivity of cathode, conductive polymer polypyrrole (PPy) was electrochemically coated on the surface of crystalline LiV_3O_8 particles in the acetonitrile medium to produce LiV_3O_8/PPy composite film. With composite polymer electrode, the morphology, including the size, of LiV_3O_8 crystal particles is also playing critical role in battery performance. In this work, two different types of crystalline LiV_3O_8 particles – (i) nano-size resulted from solution evaporating method and (ii) micro-size resulted from solid state reaction method – are investigated. These new materials were characterized by X-ray diffraction spectroscopy, scanning electron microscopy, FTIR spectra, and battery tester. It was found that PPy were grown uniformly on the surfaces of the crystalline particles of both kind. However, the attributions of PPy incorporated within the composite films are different, and so are the battery performances.

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Battery Performance of $LiFePO_4$ coated with p-TSA doped PEDOT

Hung-Cuong Dinh, *엄광섭, **여인형, ***조원일, 모선일

*아주대 에너지시스템학부 *아주대 NT.IT Fusion Tech **동국대 화학과 ***KIST 에너지환경연구부*

$LiFePO_4$ is one of the promising cathode materials for Li-ion batteries, due to its thermal stability, environmental benignness, attractive voltage ca. 3.5 V, high theoretical capacity (170 $mAhg^{-1}$), and low cost. However, it exhibits low conductivity (~ $10^{-9}Scm^{-1}$) which is a critical disadvantage as battery electrode. In order to increase the electronic and ionic conductivity, much effort has been made such as changing crystalline $LiFePO_4$ particle size (nano-scale), coating conductive carbon, adding metals/metal oxide on the surface of the particles, or doping supper-valance ions in crystalline lattice. In this work, conducting polymer PEDOT doped with p-TSA was synthesized and used to produce composite films embedding the crystalline $LiFePO_4$ particles. Micron-/nano-sized $LiFePO_4$ particles were synthesized by a hydrothermal method and they were coated with conducting polymer PEDOT doped with p-TSA. The $LiFePO_4$ powder is dispersed in polymer solutions and dried in vacuum at 80oC for 1 day. After assembling Li coin cells, cathode performances were examined by charge-discharge cycle test and cyclic voltammetry (CV) using a multichannel battery tester. The rechargeable battery cycle stabilities and specific capacities of micron-/nano-sized crystalline $LiFePO_4$ particles coated with conducting polymer PEDOT doped with p-TSA are presented.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

V_2O_5 and PEDOT composite films doped with various contents of p-TSA

송한목, Quang-thao Ta, *엄광섭, **여인형, 모선일

*아주대 에너지시스템학부 *아주대 NT.IT Fusion Tech **동국대 화학과*

Nano-sized V_2O_5 has been investigated as one of the promising cathode materials in rechargeable lithium batteries due to the advantages of high voltage, large surface area, short diffusion path of Li-ion. However, its critical disadvantages are low conductivity and large volume variations during the battery cycles. Polymer poly3,4-ethylenedioxythiophene (PEDOT) is one of the most successfully conjugated conducting polymers in solving these disadvantages, since it has high conductivity, mechanical flexibility, and environmental stability. However, in contrast to polypyrrole, PEDOT cannot receive oxidative catalytic action of V_2O_5 for the polymerization, while this action is needed for the smooth surface coating of V_2O_5 during the electrochemical polymerization at the electrode surface to form the electrochemically produced V_2O_5/PEDOT composite film. This work demonstrated that the doping of para-toluenesulfonic acid (p-TSA) into the composite film by adding p-TSA in the electrolyte can induce smoother coating and also increase the conductivity of PEDOT. The characteristics of V_2O_5/PEDOT composite film with various p-TSA doping, together with the performance of the battery cathode, have been investigated using the methods of FT-IR, SEM, cyclic voltammetry(CV), impedance measurement, and battery test.

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Synthesis and Luminescence Properties of Double Perovskite $Ba_2Bi_{2/3}TeO_6:Eu^{3+}$ Orange-Red Phosphors

Nguyen Hoang Duy, *엄광섭, **여인형, 모선일

*아주대 에너지시스템학부 *아주대 NT.IT Fusion Tech **동국대 화학과*

The phosphor coverted white light-emitting-diodes (LEDs) have received much attention due to their advantages, such as brightness, reliability, power efficiency, and lifetime. The white LED has been initially fabricated using blue LEDs and yellow-emitting phosphor. However, it lacks red component in the spectra and has low color-rendering index (CRI). The red-emitting phosphor has also been introduced to improve the CRI and increase the light conversion efficiency. In this study, a new orange-red emitting phosphor of double perovskite $Ba_2Bi_{2/3}TeO_6$doped with Eu^{3+} was synthesized by solid stated reaction method. Morphology, crystal structure, and optical properties of the phosphors were examined by a scanning electron microscopy (SEM), powder-XRD and a spectrofluorometer. The phosphor presented a broad excitation band in near UV range (350-470 nm). The emission spectra performed two peaks at about 595 nm and 615 nm arising from the $^5D_0$-$^7F_1$- and $^5D_0$-$^7F_2$ transition of Eu^{3+},respectively. The intensity of charge transfer and its orange-red emission have increased about 30% by using Na_2S_x flux in synthesis process. The effect of Eu co-doping concentration and the utilization of Na_2S_x flux on the emission characteristics of the $Ba_2Bi_{2/3}TeO_6:Eu^{3+}$ phosphors are investigated and discussed.

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리튬 이차전지용 분리막의 젖음성 결정인자 규명

손화영, 이호춘

금오공과대 응용화학과

리튬 이차전지용 분리막의 전해액에 대한 젖음성 (wetting) 특성은 리튬 이차전지 성능에 중대한 영향을 미치며, 또한 전지의 생산속도를 결정하는 중요한 요소이다. 이러한 중요성에도 불구하고, 이제까지 분리막의 wetting 특성에 대한 연구는 매우 미진한 실정이며, 특히 전해액의 조성과의 상관관계에 대한 연구는 거의 전무한 실정이다.분리막의 wetting 특성은 분리막의 이온전도도에 영향을 주며, 이는 다시 분리막과 전해액의 종류에 영향을 받게 된다. 본 연구에서는 신뢰성이 높은 분리막 이온전도도 측정법을 확립하고, 이를 이용하여 분리막의 wetting 특성에 대한 상기 변수들을 규명하고자 한다. 즉, 분리막의 제조방식 (건식법 vs. 습식법), 분리막의 제조변수 (재료, 기공도, 기공크기), 및 전해액의 조성변수(염의 농도, EC 함량)등이 분리막의 wetting 특성에 주는 영향을 규명하고자 한다.

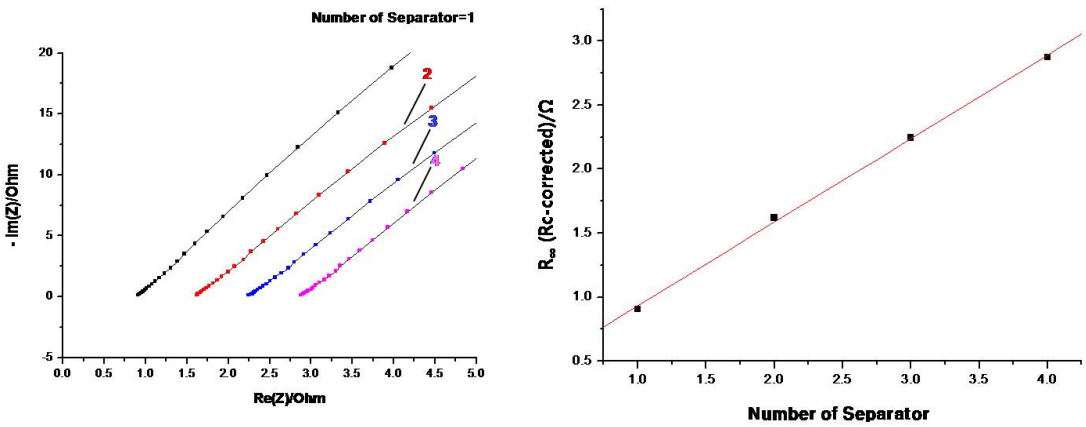

Fig1. 분리막 수에 따른 **Nyquist plot** (왼쪽)과 **ionic resistance** 관계 그래프(오른쪽)

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Influence of ternary mixed solvent electrolyte on electrochemical properties of LiFePO4 cathodes for rechargeable lithium cell

배준우, 이호춘

금오공과대 응용화학과

A novel solvent, KCS-1, for improving rate performance of the lithium-ion battery (LIB) has been presented. 1M LiPF6 ethylene carbonate, dimethyl carbonate, and KCS-1 (EC/DMC/KCS-1) shows 10-20% higher ionic conductivity than the electrolyte without KCS-1. The Li/LiFePO4 cell retains 60% of the discharge capacity at 5C rate with KCS-1, while it only keeps 25% of discharge capacity without KCS-1.Anodic stability of KCS-1 is comparable to carbonates until 4.6V (vs. Li+/Li), which is applicable to LIBs. The compatibility of the KCS-1 with graphite anode is not quite good, but it can be much improved by using SEI-forming additives such as VC and FEC. In brief, KCS-1 is promising as the electrolyte solvent or the high power LIBs for HEV, EV, and power tools.

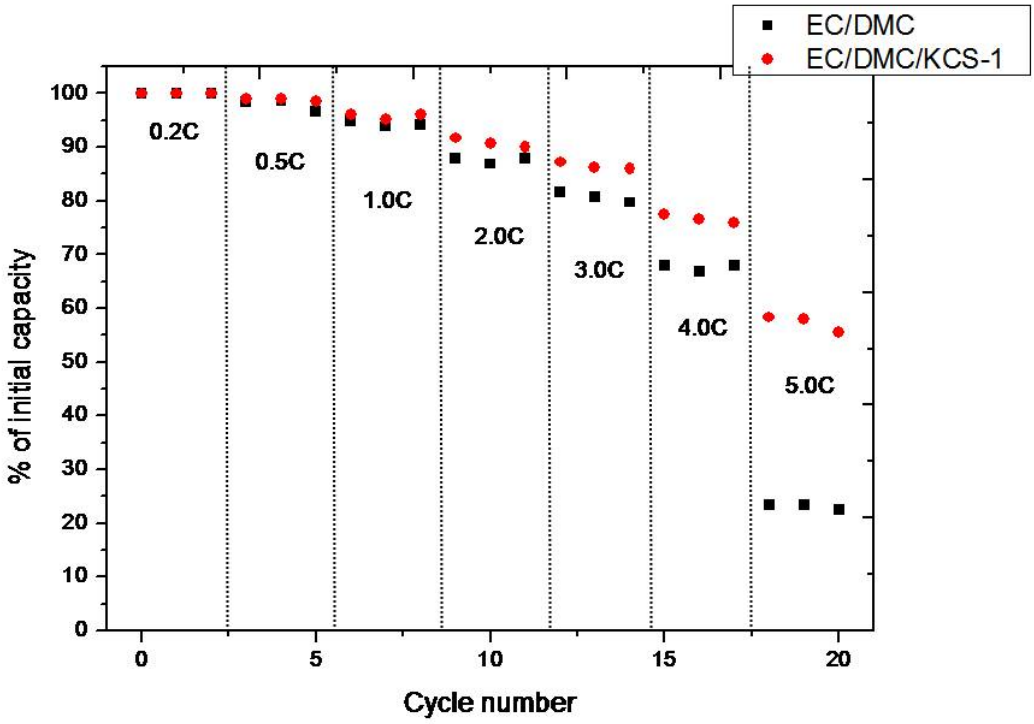

Fig.1. Rate capability of the lithium-ion cell with the KCS-1 or the without KCS-1 as a function of cycle number.

THE KOREAN CHEMICAL SOCIETY

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Aptamer selection based on target immobilization on conducting polymer film

김유정, 노희복, **Pranjal Chandra**, 탁성희, 심윤보

부산대 화학과

Aptamer, as a new class of single-stranded oligonucleotides, obtained by the method called “systematic evolution of ligands by exponential enrichment (SELEX)” from random RNA or DNA libraries. In this study, we report aptamer selection based on target immobilization on conducting polymer film at screen printed electrode. Thrombin was used as a standard target protein in present work. At first stage thrombin was immobilized on SPCE/polyTTCA film by covalent bonding. Immobilization of protein, and further thrombin/polyTTCA/SPCE interaction with aptamer/oligonucleotides was confirmed impedance spectroscopy. Same experimental conditions will be performed and interaction between DNA library and Thrombin/polyTTCA/SPCE will be done. Dissociation constant of standard thrombin aptamer and designed aptamer by our method, for thrombin interaction will also be confirmed.Keywords: Aptamer; SPCE; Thrombin; SELEX

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염료감응 태양전지용 pyridinium iodide 계열의 무용매 이온성 액체 전해질 및 무용매 Silica-이온성 액체 복합 겔 전해질

전세미나, *한치환, 김강진

*고려대 화학과 *한국에너지기술연구원 광전기소재연구센터*

염료감응 태양전지(DSSC)은 광합성원리를 이용한 고효율의 광전기 화학적 태양전지로 1991 년 스위스 EPFL 의 Grätzel 그룹에서 11.1%의 광전변환 효율을 보고하였다. 이는 액체 전해질을 사용하는 염료감응 태양전지로 구성성분인 용매(acetonitrile 등)의 증발 가능성에 의한 전해질의 누수로 전지의 장기 안정성을 보장할 수 없어 상용화하는데 어려움이 있다. 이러한 약점을 극복하고자, 고체 상태의 정공-전달체(저분자 유기물 혹은 공액고분자)를 사용하거나 겔 상태 또는 고체 상태의 고분자 전해질을 사용하여 액체 전해질을 대체하고자 하는 노력이 시도되고 있으며, 중국과학원(Chinese Academy of Sciences)의 Peng Wang 박사 연구팀은 용매 없이 imidazolium iodide 계열의 이온성 액체를 이용하여 8.2%의 에너지 변환효율을 발표했다. 본 연구에서는 우수한 화학적, 열적 안정성, 고이온 전도성 및 낮은 증기압을 가지는 이온성 액체인 pyridinium iodide 계열을 이용한 무용매 이온성 액체 전해질을 연구하였다. 또한 pyridinium iodide 계열의 무용매 이온성 액체 전해질에 나노 Silica 를 blending 하여 Silica-이온성 액체 나노 겔 전해질을 만들어 염료감응 태양전지에 적용하였다.

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Aptamersensor for chloramphenicol detection

Pranjal Chandra, Ye Zhu, 노희복, 심윤보

부산대 화학과

A chloramphenicol (CAP) aptamersensor was fabricated by covalent immobilization of aptamer on carbon nanotube-doped conducting polymer (poly 5, 2′: 5′, 2″-terthiophene-3′-carboxyl acid (poly-TTCA)) layer electropolymerised on GC/AuNP surface. The AuNPs, MWCNT were used in order to enhance the sensitivity of the sensor probes. The particle sizes were determined using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The immobilization of aptamer was confirmed using, X-ray photoelectron spectroscopy (XPS), and quartz crystal microbalance (QCM) techniques. The detection was based on direct electrochemistry of CAP. Various experimental parameters, pH, temperature, applied potential, aptamer concentration and deposition time were optimized and performance of the CAP aptamer sensor was examined. The fabricated aptasensor exhibited a wide dynamic range of 1x10-8 and 10x10-7 M and a detection limit of CAP of 7x10−9 M (k = 3, n = 5). Further the selectivity and real sample analysis will be done using rat bone marrow tissues.Keywords : Aptamersensor; Chloramphenicol

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Fabrication of a MIP-based glucose sensor

Juehan Gao, Ye Zhu, 심윤보

부산대 화학과

A novel electrochemical sensor coated with molecular imprinted polymers (MIP) has been developed for the determination of glucose. To fabricate a stable sensor probe, we modified the probe surface with a conjugated polymer (5,2′:5′,2′′-terthiophene-3′-carboxylic acid, TTCA), which serves as a base substrate to construct the artificial biomembrane. The AuNPs were electrodeposited onto a glassy carbon electrode (GCE). A layer of glucose-MIP was photochemically grafted over the poly-TTCA/AuNPs/GCE. The molecularly imprinted sensor was characterized by EIS impedance spectroscopy, differential pulse voltammetry (DPV), Atomic force microscopy (AFM), X-ray photoelectron spectroscopy(XPS) and cyclic voltammetry (CV). The MIP artificial sensor showed high sensitivity, selectivity, and reproducibility.Keywords: Molecular imprinted polymers (MIP); Glucose; Sensor

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Detection of An Antibiotic by Aptamer Immobilized on Conducting Polymer / Gold Nanoparticle Composite

Ye Zhu, Pranjal Chandra, koh wei choon alvin, 심윤보

부산대 화학과

In the present work, an aptamer sensor for an antibiotic was developed based on gold nanoparticles and poly-[2, 5-di-(2-thienyl)-1H-pyrrole-1-(p-benzoic acid)] (pDPB) layer modified glassy carbon electrode. The probe was prepared by immobilizing specific aptamer onto the conducting polymer through covalent bond. The modification of the electrode surface was characterized using scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). The capturing of antibiotic by the prepared probe was demonstrated by cyclic voltammetry and differential pulse voltammetry. The cyclic voltammograms showed a pair of redox peaks at 210 / 35 mV at aptamer modified surface. The parameters that could affect the response, such as aptamer concentration, incubation time, temperature, and pH were optimized. Different concentrations of the antibiotic were detected, and the calibration plot was obtained consequentially.Keywords: Conducting polymer; Gold nanoparticle; Aptamer sensor; Antibiotics

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Determination of Cytochrome C with Cellulose – DNA modified Screen Printed Carbon Electrodes

정진욱, 정새로미, 심윤보

부산대 화학과

A sensor for cytochrome c (cyt c) was developed using a screen printed carbon electrode (SPCE) modified with cellulose-DNA. cyt c was adsorbed on the cellulose-DNA modified SPCE through the electrostatic interaction between them. Owing to this process, a pair of well-defined peaks appeared at 48 mV/85 mV (Epc/Epa vs. Ag/AgCl). This property of the cellulose-DNA modified SPCE was utilized for the analysis of cyt c in a biological sample. The optimum experimental conditions for analysis were investigated and a calibration plot was obtained between 3.1X10-6 M and 4.0X10-7 M at the optimized condition. The real sample analysis was carried out with the standard addition method to evaluate the developed method. The content of cyt c in cancer cell in mitocondria fractions was determined.Keyworlds : DNA senso; Cytochrome c; Screen printed carbon Electrode; DPV

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Electrocatalytic reduction of carbon dioxide on Au-Zn alloy dendrite modified glassy carbon electrode

최영진, 노희복, 김동민, 심윤보

부산대 화학과

Au-Zn alloy dendrite was formed on a glassy carbon (GC) electrode by electrodeposition. The solution were in water with 0.1M KH2PO4 as the supporting electrolyte. Zn2+ ion can reduce underpotential condition both existence gold(111) and phosphate ion. This phenomenon can occur by Zn-PO4 complex. The dendrite material was characterized by employing SEM, XPS and EDS. It was observed that the Au-Zn alloy dendrite had excellent catalytic ability in the reduction of carbon dioxide as compared with Au dendrite and Zn dendrite. To evaluate the catalytic properties of the dendrite in the reduction of carbon dioxide, cyclic voltammograms (CVs) were recorded for bare GC, Au, Zn, and Au-Zn alloy dendrites in CH3CN/LiClO4 solution.

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The effect of Carbon coated $Li_4Ti_5O_{12}$ using chitosan for the Lithium ion secondary batteries

한현주, *진종성, 정옥상, **도칠훈, *정의덕

*부산대 화학과 *한국기초과학지원연구원 하이테크부품소재연구부 **한국전기연구원 전기재료연구본부 전지연구센터*

The $Li_4Ti_5O_{12}$ powders were synthesized by using the sol-gel method with Lithium acetate, Titanium isopropoxide and chitosan as a carbon precursor material for a cathode of a lithium-ion battery. The chitosan added $Li_4Ti_5O_{12}$ powders were calcined at 400℃ for 6 hours and then calcined at various temperatures (650℃, 750℃ and 850℃) in air atmospheres for 2 hours respectively. We characterized the synthesized compounds via the crystallinity, confirm of carbon, atom image mapping and their shapes using TGA, XRD, SEM-EDS, TEM, XPS and Nano SIMS. We found that the synthesized powders were carbon-coated using Nano-SIMS and TEM images. We observed voltage characteristics and initial charge-discharge characteristics according to the C rate in $Li_4Ti_5O_{12}$ electrodes. The obtained initial specific capacity of the chitosan added $Li_4Ti_5O_{12}$ powder was 112mAh/g with excellent cycle stability which is much larger than that 98mAh/g of pure $Li_4Ti_5O_{12}$ powder at 0.1C rate.

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Electrocatalytic water splitting with Co3O4 films prepared by a paste coating

전효상, *민병권

*과학기술연합대학원대 청정연료 화학공학 *KIST 청정에너지연구센터*

Direct electrochemical water splitting is a non-polluting way of producing pure hydrogen. Particularly, the products are free of CO, which is very beneficial in fuel cell applications. In the electrochemical water splitting, the obstacle would be an anodic reaction for oxygen evolution where substantial energy loss occurs mainly due to the high overpotential. Numerous electrocatalysts have been applied to reduce the overpotential in the water splitting including expensive precious metals (e.g. Ir, Ru, and Rh). In this study, we focused on the development of electrocatalyst with low cost ways: inexpensive material as well as low cost coating method. We demonstrate successful fabrication of Co3O4 electrocatalyst films at low temperature (′ 50 oC) on a stainless steel substrate by a paste coating method using Nafion as a binder. The Co3O4 films were found to be catalytically efficient in water splitting reaction in an alkaline aqueous solution. In addition, we elucidated the relationship between the electrocatalytic activities and the particle size of Co3O4 in water splitting reaction. The details will be discussed in the presentation.

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Determination of glucose based on glassy carbon electrode by glucose oxidase and MWCNT-palladium nanoparticles

유정민, 김슬기, 설희진, 김대근, 전승원

전남대 화학과

We have developed and characterized the performance of a glucose biosensor based on glucose oxidase (Gox) with cross-linking in the matrix of bovine serum albumun (BSA), and MWCNT-palladium nanoparticles. The Nafion/God /MWCNT-pd/GCE was easily prepared in a rapid and simple procedure, and it application is improved the sensitive of determination glucose. Meanwhile, the results obtained from each CV, amperometric methods for glucose determination were comparable. Based on the result of the amperometric method, the respond time was very short, and the line are egressione quation was obtaine the very low concentration region of less than 1.0 mM at an applied potential of 0.4 V. The glucose was determined at an applied potential of 0.4 V by amperometric method. It was found that the line arresponse for glucose was from 1 μM to 10 mM. The resulted sensor shows fast response and good stability.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ELEC.P-66**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Electrocatalytic reduction of oxygen at CoTAPP-Pd/SWCNT coated GCE electrode

MohammadShamsuddin, 유정민, 전승원

전남대 화학과

The influence of polymeric cobalt-tetrakis(2-aminophenyl)porphyrin (CoTAPP)-Pd films on the kinetics of dioxygen reduction was investigated using SWCNT/Nafion coated glassy carbon electrode (GCE). A rotating ring-disk electrode (RRDE) technique was used to determine kinetic parameters for O2 reduction and to detect intermediate H2O2 formation. Kinetic parameters such as the kinetic current, Tafel slope, potential dependence of the ratio of the direct 4-electron reduction to the series 2-electron reduction were determined in 0.1 M H2SO4. The kinetic data showed the clear evidence of the enhancement effects of SWCNT/Nafion coating on the cathodic O2 reduction at GCE. This suggested that our proposed modified electrode Nafion/CoTAPP-Pd/SWCNT/GCE is good candidate for catalytic reduction of dioxygen.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **ELEC.P-67**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

A Selective determination of hydrogen peroxide on SWCNT, Poly(EDOP) and palladium nanoparticle coated GCE

김대근, 유정민, 김슬기, 정대철, 전승원

전남대 화학과

We developed a hydrogen peroxide biosensor of glassy carbon electrode. The activity of P(EDOP)-Pd/SWNT nanoparticles based on modified glassy carbon electrode for the detection of H2O2 was investigated using cyclic voltammetry in phosphate buffer saline (PBS) solution at pH 7.4. The resulted sensor fast response and good stability.

THE KOREAN CHEMICAL SOCIETY

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDEC.P-1**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중학교 과학 교과서 내 화학 단원에 나타난 질문 형식의 문장 분석

허만규, *최은주, *오영희

*동의대 분자생물학과 *동의대 화학과*

본 연구는 중학교 과학 교과서 17 종을 대상으로 화학 단원 본문 내용 중에 제시된 질문을 빈도, 양식, 위치 등에 따라 비교 분석하였다. 조사 도구는 캘리포니아 대학에서 1975 년 협동적 교사 준비 프로젝트의 일환으로 개발된 교과서 질문 방략 평가도구(Text Questioning Strategies Assesment Instrument: TQSAI)를 사용하였다. 전체 문장 중에서 질문이 함유된 문장의 비율을 구하고 질문의 위치 분석을 통하여 다양한 질문이 마지막 단계를 제외하고 제목과 초기단계와 전 교과서 내용에 설정되어 있었음을 알 수 있었다. 또한 탐구성 분석, 질문의 구성도 분석, 경험 관련도 분석 등과 다양도 지수등의 정량분석에 의한 각종 지수등을 조사 분석하였다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDEC.P-2**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중학교 과학 교과서 내 화학 분야의 단원정리 문항의 분석

허만규, *오영희, *강경남

*동의대 분자생물학과 *동의대 화학과*

2010 년 중학교 검인정 과학 교과서 전체 17 종을 대상으로 화학 단원에서 제시된 정리 문제에 대한 문항 분석을 실시하였다. 17 종 교과서 중 1 개 교과서(3 개 단원)를 제외하고 4 개 단원에 화학 분야를 설정하고 있어 그 단원을 대상으로 연구하여, 인지 수준에 따른 문항 분석, 형식에 따른 문항분석, 과학적 탐구영역에 관한 문항분석을 하였다. 그리고 단원 간 유사한 빈도를 유지하고 있는지에 대하여 카이자승 검정과 항목 간 분산의 정도 등을 조사하였다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDEC.P-3**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

일반화학에서 ConcepTests의 활용이 학업 성취도와 학습태도에 미치는 영향

문숙희, 이상좌

목포대 화학과

이 연구는 ConcepTepts 를 활용하여 학생들을 일반 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 1 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.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDEC.P-4**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

과학고등학교 심화화학 교재 개발을 위한 외국 사례의 분석

백종호, 정대홍, *이진승

*서울대 화학교육과 *서울고*

제 7 차 교육과정에서 2009 개정 교육과정으로 전환되면서 과학고등학교의 수업과정에도 변화가 생기게 된다. 기존의 교육과정의 전문교과에 해당하는 각 교과의 '과학Ⅱ','고급과학'과목이 '고급과학', 대학과목을 선 이수하는 'UP 과목'으로 재편성 되었다. 이에 따라 1 학년 때 학습하는 보통교과에 편성되는 과학교과를 제대로 이수하지 못할 우려가 있어 기존의 '과학Ⅱ'와 실험과목을 압축, 심화하여 보통교과의 과학 과목을 보완하는 역할의 '심화과학'과정이 새로 신설되었다. 심화과학은 보통교과와 전문교과(고급과학), UP 과목 등의 학습 계통성을 유지할 수 있는 연계과목으로서의 역할을 수행하게 된다. 이 중 심화화학은 학생들에게 화학에 대한 이해와 체계성을 높여줘야 할 필요성이 있기 때문에 화학의 이론과 화학 실험을 동시에 경험하는 것이 필요하다. 제 7 차 교육과정에서는 화학의 이론과 화학실험을 분리하여 운영하였지만, 과학적 사고력의 향상을 위해 다양한 탐구과정을 수반하는 형태로 심화화학 교재의 개발이 필요하다. 새로 개발되는 심화화학은 다양한 탐구 과정을 통한 과정 지식과 개념의 획득을 목표로 하고, 이를 통해 학습 과정 중에 문제 해결 능력, 과학적 사고력의 신장을 이루어 학생의 창의력 신장을 최종 목표로 해야 한다. 이 연구는 과학고등학교에서 사용할 교재로서 과정과 다양성을 추구하며 화학 이론과 실험을 통합한 형태의 심화화학 교재 개발을 위해 기존의 '화학Ⅱ'의 내용요소를 추가, 변경하여 '심화화학'교재의 내용요소를 도출한 내용을 담고 있다. 새로이 개발되고 있는 심화화학은 '물질변화와 에너지', '화학 평형'. '화학 반응 속도론'등의 총 9 개의 대단원으로 구성되어 있다. 단원의 순서는 단원 내용의 흐름에 따라 자연스럽게 연계되도록 구성하였고, '양의 표현과 측정', '분리와 분석'과 같이 학생들이 실제 과학실험, 활동을 진행할 때 필요한 지식 및 방법을 담아내었다.

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장소: 대구엑스코
발표코드: **EDEC.P-5**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중고등학생, 예비 과학교사의 나노과학에 대한 인식 조사 및 교육 자료의 개발

윤희숙, *이준규, 강성준

*강원대 과학교육학부 *강원대 사범대학 과학교육학부 화학교육전공*

현대의 과학기술은 앞을 예측할 수 없을 만큼 빠르게 발전하고 있다. 특히 첨단 과학 기술 분야는 그 발전 속도가 워낙 빨라 일반 사람들이 따라갈 수 없고 파악할 수 없을 정도이다. 이러한 첨단 과학 기술 중에서도 근래에는 나노 관련 제품들이 많이 출시가 되면서 생활 속에서 나노 제품과 접할 기회가 많아졌다. 그로 인해서 많은 학생들이 '나노'라는 말을 들어보았지만, 정작 나노가 정확히 어떠한 개념인지 또한 나노기술이 어떠한 것인지 잘 알지 못하며, 국내 중고등학교에선 아직도 나노기술의 잠재력에 대한 교육이 사실상 전무한 실정이다. 본 연구의 목적은 중, 고등학생, 예비 과학교사의 나노에 대한 인식이 어떠한 지 알아보고 학생들에게 적합한 나노 교육 자료를 개발하는 것이다. 이를 위해 먼저 중소도시의 중 ,고등학생, 과학 예비교사를 대상으로 나노과학에 대한 인식을 묻는 설문조사를 실시하였다. 설문조사 결과 일부의 학생들만이 비교적 정확한 개념을 가지고 있었으며, 나노과학에 대한 정보는 주로 인터넷을 통해 얻고 있었다. 응답자들은 나노과학의 긍정적인 측면에 대한 인식을 가지고 있었으며, 나노과학의 위험성에 대한 인식은 낮았다. 이러한 점을 개선하기 위하여 '나노'에 대한 개념과 우리생활과의 관계를 알려줄 수 있는 자료, 은나노입자의 제조와 나노용액의 성질을 알아보는 탐구실험, 직접 신문의 기사를 통해서 나노의 장 ,단점에 대하여 서로 토론할 수 있는 자료를 바탕으로 중등학생이나 예비과학 교사를 위한 나노과학 교육자료를 개발하였다.

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장소: 대구엑스코
발표코드: **EDEC.P-6**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중,고등학교 수업에서 활용 가능한 증기 압력 측정 실험의 개발

윤희숙, *김지명, 김아름

*강원대 과학교육학부 *강원대 사범대학 과학교육학부 화학교육전공*

증기 압력과 액체의 끓음 현상은 학생이 일상생활의 경험을 통해 자주 접하고 있는 자연 현상이지만 액체에서 눈으로 관찰할 수 없는 기체 상태로의 변화를 다루므로 학생이 올바른 과학적 개념을 갖기가 어려운 현상 중의 하나이다. 선행 연구에 의하면 학생들은 증발과 끓음을 구별하는데 기화 위치나 기포 발생과 같은 과학적 개념보다는 가열 여부로 판단하여 가열하지 않으면 증발, 가열하면 끓음이라고 인식하고 있는 것으로 나타났다. 본 연구의 목적은 끓음과 증기압력을 측정할 수 있는 간단한 장치의 고안을 통해 중고등학교 교육과정에서 제시되고 있는 관련개념의 학습에 도움이 되는 실험자료를 개발하고자 하는 것이다. 이를 위해 MBL 장치와 압력계 달린 진공용기를 이용한 두 종류의 증기 압력 측정 실험을 고안하였다. 고안된 장치를 이용한 실험 결과 모두 압력이 감소함에 따라 끓는점이 감소하는 경향을 보였으며, 장치를 이용한 측정값은 이론값과 비슷하였다. 또한 실험값을 통해 에탄올과 물의 증기압을 비교해 보았는데 같은 압력에서 물의 끓는점이 에탄올보다 높고, 같은 온도일 때 에탄올의 증기압이 물보다 높다는 결과도 얻을 수 있었다. 이 장치는 끓음과 압력과의 관계, 온도에 따른 증기압력의 변화, 물과 에탄올의 혼합물의 증기압력을 측정할 수 있는 실험에 사용될 수 있다. 각각의 증기 압력과 끓는점에 관한 실험 수업에 활용할 수 있도록 학생 활동지와 교사용 지도 자료를 개발하였다.

일시: 2010년 10월 14~15일(목~금) 2일간
장소: 대구엑스코
발표코드: **EDEC.P-7**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

포화 용액 개념에 대해 초등학교 교사들이 만든 비유의 분석

강훈식

춘천교육대 과학교육과

이 연구에서는 포화 용액 개념에 대해 초등학교 교사들이 만든 비유를 비유의 개수, 소재, 유형 측면에서 분석했다. 또한, 그 결과를 초등학교 일반 및 과학영재 학생들의 결과와 비교했다. 초등학교 교사 111 명을 대상으로 비유 만들기 검사를 실시했으며, 일부 교사들을 선정하여 심층적인 집단 면담도 실시했다. 연구 결과, 일반 및 과학영재 학생들보다 교사들이 더 많은 수의 비유를 만드는 것으로 나타났다. 전반적으로 교사와 학생들 모두 가정 상황, 탑승 상황, 소화 상황, 학교 상황 소재를 사용하여 비유를 만드는 경향이 있었으나, 신체/신체 활동 상황, 환경 상황, 생물 상황을 포함한 이외의 소재 상황을 사용하여 만든 비유의 경우에서는 교사와 학생들 사이에 약간 차이가 있었다. 학생들의 경우와 유사하게 교사들은 구조적 또는 구조적/기능적 비유보다는 기능적 비유를, 추상적 비유보다는 구체적 비유를 더 많이 만들었다. 반면, 교사들은 학생들보다 글 비유, 작위적 비유, 부연 비유를 더 많이 만들었으며, 고체계성 비유의 경우에는 일반 학생들보다는 더 많이, 과학영재 학생들보다는 더 적게 만들었다. 이에 대한 교육적 함의를 논했다.

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멘토링을 통한 초임 초등교사의 반성적 교수실행 변화

공영태, *이정현

*진주교육대 과학교육과 *진목초등학교 교사*

이 연구에서는 교수실행에 대한 반성적 사고와 반성적 실천을 유도하는 협력적 멘토링을 통하여 초임 초등교사의 과학수업에서의 수업 및 인식에 있어서의 변화를 알아보았다. 연구 참여자는 2 명의 멘토 교사와 2 명의 멘티 교사, 대학교수 1 명, 수업분석자 3 명, 본 연구자 등 총 9 명으로 구성되었으며, 교직 경력 1 년 이하의 멘티 교사 2 명을 멘토 교사와 일대일로 2 개 팀을 구성하여 7 개월간 5 차례의 멘토링을 실시하였다. 이 과정에서 멘티수업 녹화본 및 전사본, 학습지도안, 일대일 멘토링 녹음 및 전사본, 멘티 저널, 교수관찰지(RTOP) 등의 자료를 수집하였다. 7 개 그룹으로 이루어진 교수관찰지를 수업 분석에 이용하였으며, 멘티 교사의 수업에 있어서의 인식과 변화는 저널과 일대일 멘토링 면담자료를 통해 알아보았다. 멘티 교사들의 멘토링 전 수업은 학생 탐구활동이 이루어지지 않은 교사 위주의 강의식 수업으로 7 개 그룹의 모든 교수행위 도달도가 매우 낮은 것으로 나타났다. 교과내용지식과 관련된 측면은 어느 정도 구성되어 있으나, 학생들에게 다양한 탐구활동의 기회를 제공해주는 탐구적 교수법과 학생들의 능동적 지식 구성을 강화하는 수업방법에 있어서는 매우 취약함을 보여주었다. 실제 수업에서의 멘티 교사들에게 공통적으로 나타난 특징은 교사의 발문 기술 부족으로 인한 학생과의 상호작용 부족, 학생의 학습 곤란도와 학습 정도를 파악하려는 평가와 관련된 교수 전략의 부재, 교사 주도의 지루한 강의식 수업과 어수선한 교실 분위기, 교사의 인내심 부족, 실험수업 기피 경향 등을 들 수 있다.

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TIMSS 2007 초등과학 화학분야 문항 분석

공영태, *노민해

*진주교육대 과학교육과 *사천 남양초등학교 정보부*

이 연구는 TIMSS 2007 초등학교 과학 공개 문항(63 문항)을 번역하여 우리나라 초등학교 4 학년 아동들에게 적용하고, 이들 가운데 화학분야 문항에 대한 우리나라 아동들의 성취 결과를 알아보고자 하였다. 각각의 공개 문항별 우리나라 학생들의 정답률을 살펴보았고, 이를 국제 평균치와 비교하였다. 또한, 제 7 차 과학교육과정과의 관련성을 파악하며, 새로운 과학교육과정 개정에 있어서 시사점을 제시하고자 하였다. 이번 연구를 통해 다음과 같은 몇 가지 결론을 도출할 수 있다. 첫째, TIMSS 2007 초등 화학 공개 문항과 제 7 차 초등학교 교육과정을 비교 분석함으로써 현 교육과정과의 관련성을 파악할 수 있었다. 둘째, TIMSS 2007 초등 화학 문항에서 다루는 학습내용의 이수시기를 파악할 수 있었다. 셋째, TIMSS 2007 초등 화학 문항의 이수 여부에 따른 정답률과 학생들의 응답 반응을 파악할 수 있었고, 이에 따라 교육과정의 개정 및 지도방향을 모색할 수 있었다. 넷째, 화학분야에 대한 우리나라 초등학생의 정답률 평균은 62.7%로 생물과 지구과학영역에 비하여 높은 정답률을 나타내었다. 다섯째, 선다형의 정답률이 서술형의 정답률보다 높게 나타났다.

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TIMSS 2007 초등 과학문항의 성취수준별 문항 분석

공영태, *김수희

*진주교육대 과학교육과 *마산 호계초등학교*

이 연구에서는 TIMSS 2007 에서 국제적 표준으로 선정되어진 문항들을 중심으로 우리나라 초등학생이 보여주는 정답률을 살펴보고 이러한 정답률의 원인 분석을 교육과정 이수 및 학생들의 오개념의 관점에서 고찰하고자 하였다. 우리나라는 지난 TIMMS 2003 뿐만 아니라 이번 TIMSS 2007 의 조사에 초등학생들은 참석하지 않았다. 따라서 우리나라 학생들에 대한 기초적인 자료를 수집하기 위하여 TIMSS 2007 에서 공개된 문항을 가지고 2009 년에 경남 소재 초등학생들 500 여명 대상으로 조사를 행하였다. 이 연구를 통하여 초등학교 4 학년 아동들이 가지고 있는 과학개념 인식 정도의 정확한 파악을 위한 기초 자료를 제공하는 것을 목적으로 하고 있다. 또한 이 연구는 초등학교 학생의 과학학업 성취도 변동 추이와 함께 교수학습의 실제 및 정책을 국제수준과 견주어 볼 수 있는 기회를 제공하고자 하였다. 성취수준별 문항은 국제적인 학업 성취도의 비교를 위하여 타당도 높은 중요한 요인 중의 하나이다. 따라서 이 연구에서는 주로 TIMSS 2007 에서 공개된 초등 과학 문항가운데 성취수준별이 제시되어 있는 문항들을 살펴보았다. 국제보고서에 제시된 8 문항외에도 일본교육정책연구소에서 제시된 항목을 포함하여 모두 10 문항을 분석 대상으로 하였다.우리나라 아동들은 대부분의 항목에서 국제평균치보다 높은 정답율을 나타내었다. 이는 우리나라 아동의 국제학업성취도가 알려진 것과 같은 우려할만한 사항이 아니라 국제적으로 높은 위치에 있음을 알 수 있었다.하지만 일부 문항에서는 우리나라 아동의 영역별 평균정답율보다 낮은 정답율을 나타내기도 하였다. 이수 유무에 따라 정답율이 차이를 나타내기도 하였지만, 이미 이수한 학습내용임에도 불구하고 정확한 개념정착이 보이지 않는 경우도 있었다. TIMSS 에서 다루는 문항들은 국제적으로 저학년부터 도입되고 있는 내용들이다. 이의 접근 방식과 다루는 깊이에 대한 연구조사를 통하여 우리나라 과하교육과정개정과 현장 학습지도에의 피드백이 필요하다.TIMSS 2007 의 최신 결과가

2008 년 12 월에 발표되었다. TIMSS 2003 의 결과가 발표된 2004 년의 학력 저하에 대한 우려에서 이번에는 다시 높은 학력수준으로 회귀하였음을 중학교 학생들의 결과로부터 확인되었다. 이는 교실내의 경쟁에 의한 결과가 아니라 여유 있는 가운데 학생들의 교육에 대한 성과가 이제서야 결과로서 나타나고 있다. 과학교육에도 경쟁을 도입하게 된 근원적인 원인이 되었던 과학학력 저하는 어쩌면 일시적인 현상이 아니었던가에 대해 좀 더 지켜볼 필요가 있다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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과학 탐구 과정에 대한 예비교사들의 인식 조사

공영태

진주교육대 과학교육과

2007 년에 개정된 과학교육과정은 과학 탐구 과정을 기초탐구과정과 통합탐구과정으로 나누어 설명하고 있다. 이는 7 차 교육과정에서의 맥락을 그대로 유지하고 있다. 하지만, 7 차 과학교과서에는 제시되어 있지 않던, 기초 탐구 과정에 대한 정의적 설명이 새로운 초등학교 과학교과서에 실려 있으며, 각 차시별 탐구 활동을 아이콘으로 표시하고 있다. 이와 같이 초등학교 단계에서부터 과학의 본성 즉 과학적 탐구 방법에 대하여 강조하고 있다. 이러한 교육의 목적을 달성하기 위해서는 현직 교사들의 이해뿐만 아니라 예비교사들의 과학적 역량을 함양하는 것이 우선적으로 필요하다. 대학 과학교육과정에서 과학의 본성에 관련된 교육과정 개정을 위한 기초적인 자료를 수집하고자 경남에 소재하는 교육대학교 1 학년, 2 학년 4 학년을 대상으로 2007 과학교육과정에서 제시하고 있는 6 가지 탐구 과정에 대한 이해도를 설문지를 통하여 조사하였다. 설문은 3 월에 이루어졌으며 자유 응답형 설문을 행하고, 필요에 따라 면담자를 선발하여 10 여분간의 면담을 행하였다. 설문지 분석결과, 연구 대상인 3 개 학년 모두 탐구과정의 정의를 올바르게 설명한 학생의 비율은 50%를 넘지 않을 정도로, 기초 탐구 과정의 정의적 개념에 대한 이해도가 부족하였다. 특히, 관찰과 측정, 예상과 추리의 개념적 차이에 대한 이해도가 부족하였으며, 서로 혼동하여 설명하는 경우가 많았다. 2 학년 및 4 학년 학생들이 가장 낮은 응답률을 나타낸 탐구 과정은 의사소통이었다. 이의 원인은 교사용 지도서에서도 의사소통에 대한 정의적 개념을 설명하고 있지 않으며 단지 교과서에서만 의사소통을 제시하고 있다. 또한 사회적인 의사소통과 과학 탐구 활동으로서의 의사소통의 차이점에 대한 구분을 짓는데 어려움을 나타내었다.

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지속가능한 발전을 위한 과학교재개발의 실천(II): 교육대학교에서의 실천

공영태

진주교육대 과학교육과

이번 연구에서는 지속가능한 발전(SD)를 위한 과학학습교재인 '대기오염대책교재'를 한국 과학교육과정에 맞게끔 재구성하여 고등학교와 대학교에 실천하였다.이번 연구에서는 지난 3 년간 교육대학교에서 이루어진 '대기오염대책교재'를 활용한 수업 교재로서의 활용성과 예비초등교사들의 응답 결과에 대하여 고찰하였다. 2008 년 8 월에는 경남 소재의 교육대학교 1 학년의 수업에 적용하였고, 2009 년과 2010 년 8 월에도 같은 내용으로 SD 과학교재의 대기오염교재를 적용하였다.교육대학교 입학생들의 대부분은 문과계열 학생들로 이번 교재의 도입부분에 해당하는 암모니아 소다법을 포함한 탄산나트륨 공업에 관한 내용이 현행 교육과정에 포함되어 있지 않기 때문에 이에 대한 사전 지식은 전혀 없었다. 나아가 이번 연구의 큰 주제어인 녹색화학(Greeen Chemistry)에 대해서도 인식도가 낮았다. 한편 2007 년 개정 교육과정에서는 지속 가능한 발전에 대한 표현이 있으며, 2009 년 개정 교육과정에서는 '녹색성장' 교과가 신설되는 등 '녹색'이 더욱 강조되고 있다.이러한 배경 가운데 1 학년 물질의 세계 수업 시간의 수업 교재로서 연구자가 직접 2 시간 수업을 행하였다.2008 년도 대학생들의 감상으로서는, '문과계출신이라서, 화학은 잘 모르지만, 유익한 시간이었다','대기오염에 대하여 내가 알고 있었던 것은 빙산의 일각이었다. 앞으로는 그린화학에 대하여 더욱 관심을 가지고 보다 열심히 배워야겠다' 등의 응답이 있었다.2009 년과 2010 년에 행한 결과를 분석하면 대부분 비슷한 응답이 얻어졌다. 미래의 예비교사로서 지속가능한 발전, 그린화학, 과학자의 역할 등에 대하여 많은 도움이 되었다는 의견이 모여졌다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

지속가능한 발전을 위한 과학교재개발의 실천(I): 고등학교에서의 실천

공영태

진주교육대 과학교육과

이번 연구에서는 지속가능한 발전(SD)를 위한 과학학습교재인 '대기오염대책교재'를 한국 과학교육과정에 맞게끔 재구성하여 고등학교와 대학교에 실천하였다.이번 연구에서는 지난 2 년간 3 개의 고등학교에서 이루어진 '대기오염대책교재'를 활용한 수업 교재로서의 활용성과 학생들의 응답 결과에 대하여 고찰하였다. 2008 년 10 월에는 경남 소재의 2 개의 고등학교에서 적용하였고, 2009 년 12 월에는 경남 소재의 4 개의 고등학교에서 SD 과학교재의 대기오염교재를 적용하였다.이번 교재의 도입부분에 해당하는 암모니아 소다법을 포함한 탄산나트륨 공업에 관한 내용은 현행 교육과정에서는 배우지 않고 있다. 또한, 대기오염이 사회적 이슈로 크게 부각된 적도 없었다. 나아가 이번 연구의 큰 주제어인 녹색화학(Greeen Chemistry)에 대해서도 그렇게 알려지지 않았다. 한편 2007 년 개정 교육과정에서는 지속가능한 발전에 대한 표현이 포함되어 지고 있으며, 2009 년 개정 교육과정에서는 녹색성장 등 '녹색'기 강조되고 있다.이러한 배경 가운데 T 고등학교에서는 2 학년 이과반과 문과반의 각 1 학급을 대상으로 연구자가 직접 2 시간 수업을 행하였다.학생들의 감상으로서는, '어느 정도 들은 적은 있지만 수업으로서 경험한 것은 처음이다. 이러한 수업은 나의 진로에 도움이 되었다','그린 화학이 무엇인가와 처음 듣는 이야기였다. 하지만, 우리들이 만든 대기오염물질에 의하여 환경이 오염되었다. 이것들을 줄이기 위하여 많은 노력을 기울여온 것을 알게 되었다' 등의 응답이 있었다.기타 고등학교에서 행한 결과를 분석하면 대부분 비슷한 응답이 얻어졌다. 그리고 이번 연구에서 함께한 교사들도 수업을 통하여 녹색화학과 과학자의 역할에 대하여 다시 한 번 고찰하는 기회를 가졌다는 등의 응답이 있었다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중학교 과학영재들의 과학 창의성 증진을 위한 화학자 폴링 따라 하기

구민아, 김지영, *박종석

*경북대 대학원 과학교육학과 *경북대 화학교육과*

과학영재들의 능력 중에서 중요하게 발현시켜야할 것으로 창의성을 들 수 있다. 창의성을 발현시키는 방법으로 여러 가지가 있지만, 과학자들이 했던 것처럼 사고하고 탐구에게 하는 것도 한 가지 방법으로 볼 수 있다. 이에 이 연구에서는 화학자 폴링의 과학적 사고과정과 탐구과정을 분석하여 이를 토대로 중학교 과학영재 교육 프로그램을 개발한다.문헌 연구를 통해 화학자 폴링의 일대기와 연구과정으로부터 폴링의 문제발견과 가설형성의 구체적인 사례를 분석하여 그의 과학적 사고를 패턴화 하고 과학영재 교육 프로그램의 구성방향을 설정한다.화학자 폴링의 연구과정으로부터 첫째, 아이디어의 생성 및 분류를 할 때 발산적 사고와 분산적 사고를 하고, 둘째, 새롭게 발견된 사례에 대해서 자신의 기존 이론으로 구조화 하며, 셋째, 그가 이룬 여러 업적은 공동연구의 결과가 많고, 넷째, 연구를 할 때 이론과 실험을 병행하며, 다섯째, 화학분야에서의 업적은 수학과 물리가 기초가 된다 등과 같은 결과를 도출할 수 있었다.이로부터 과학영재 교육 프로그램 개발을 위해 추출한 패턴은 첫째, 관점의 전환, 둘째, 귀추적 사고, 셋째, 모형화와 단순화, 넷째, 통합적사고 등이다. 이를 토대로 과학영재들을 위한 교육 프로그램을 개발함으로써 과학영재들이 창의적인 화학자 폴링의 과학적 사고과정을 따라하게 함으로써 과학탐구능력과 창의성을 증진시킬 수 있을 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중등 과학 교과서의 물질 영역에 제시된 과학적 모형들의 유형 분석

김애정, *박현주

*조선대 화학교육과 *조선대 과학교육학부*

근래 학교 과학수업이나 과학 교과서에서 여러 가지 표상들을 활용하여 학생들의 개념 이해를 도와야 한다는 주장이 강조되고 있다. 이런 표상들 중의 하나인 모형은 자연적 현상이나 과정을 묘사하는 일련의 아이디어들을 표현한 것이다. 특히 물질 영역은 비가시적이며 추상적인 개념이기 때문에 모형은 학생들이 과학 개념을 이해하는데 중요한 역할을 한다. 따라서 이 연구에서는 중등 과학 교과서에서 물질 영역에 사용되는 모형들의 유형을 분석하고 단원별로 많이 쓰이는 모형을 분석하였다. 이 연구의 대상은 2009 개정 과학과 교육과정 7 학년의 17 종 과학교과서로, 물질 분야에서 사용하고 있는 모형들을 조사하여 그 유형과 특징, 화학 내용별 특징과 빈도를 조사하여 분석하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

Analysis of Combustion Reactions of Carbon Using Microcomputer-Based Laboratory

박국태, *김동진, **민영규, **송기석, **서성일

*한국교원대 화학교육과 *병점고 **병점고 자연계열*

The purpose of this study was to analyze combustion reactions of carbon using MBL (microcomputer-based laboratory). For this study, the combustion reactions presented in high school chemistry Ⅱ textbooks were analyzed by their experimental methods. The combustion reactions using MBL were discussed on measuring reaction heat (ΔH), temperature change (ΔT), and partial pressure of oxygen (P_{O2}) change.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

고등학교 교과에서 통합교과로서의 문화재 보존과학

오진호, 정현준, 반미희

KAIST부설 한국과학영재학교

급변 할 미래사회에서는 여러 분야의 다양한 정보들을 정확하게 분석하고, 변화될 사회에 적합할 새로운 연구 분야를 만들어내는 것 필요하다. 이를 위해 여러 분야의 전문가들과 공동으로 연구할 수 있는 다 학문적 성격의 연구가 가능한 유기적 인재들의 중요성이 증가할 것이다. 이는 교육에서 각 과목 간의 경계가 조금씩 허물어지고 통합교육의 필요성이 강조되는 것과 맥을 같이한다. 20 세기에 들어와서 정립된 "보존과학"은 미래의 우수한 과학인재를 필요로 하는 새로운 연구 분야이다. 문화재 보존과학은 미래의 지도자가 될 과학영재학생들이 '문화재 가치와 상태'에 대해 올바른 이해하고, 과학 분야에서 배우는 첨단 기법들을 문화재 보존에 적용함으로써 미래사회에서 필요한 새로운 학문 분야의 개척방향을 찾게되고 더불어 문화 예술부분에 대한 의식을 고양하게 한다. 문화재 보존과학은 과학과목, 미술과목, 그리고 사회과목에 걸친 폭넓은 분야의 지식을 필요로 하는 과목이지만, 현 학교 교육과정 상에서는 각 과목 간의 연계가 부족한 현실이다. 과학기술 그 중에서도 보존과학과 가장 관련이 높은 화학기술은 급격하게 발전하고 있는데 이를 사용한 보존과학의 수업을 학생들은 접해 볼 기회조차 못 가지고 있다. 본 연구에서는 고등학교 교육과정상에서 문화재 보존과학에 관련된 과학, 미술, 그리고 사회교과의 자료 분석을 통하여 통합교과로서 보존과학 수업방안과 보존과학 수업자료를 개발하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

exploratory activities in KSASF 2010

천만석

한국과학영재학교 화학

국내외의 많은 과학축전을 통하여 탐구 능력의 향상과 상호간의 교류를 촉진하고 있다. 국내 및 국외에서 실시되고 있는 초등, 중등 과학축전의 진행과 특징에 대하여 조사하여 기초자료를 정리한다. 과학축전에서 주제탐구의 필요성과 탐구 주제내용 선정과 같은 이론적인 준비과정을 거쳐서 2010 KSA 과학축전에 참가한 학생들의 과제별 활동 모습의 소개 및 학생들의 만족도 조사와 같은 정리활동에 대해서 나누어 소개한다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중등 과학교사들의 실험에 대한 인식 조사

천희진, *박현주, **정낙주

*조선대 과학교육과(화학전공) *조선대 과학교육학부 **광주광역시교육청 교원정책과*

실험은 자연을 변인 또는 조건으로 통제.조절하고, 그 결과로 나타나는 현상들을 관찰.측정하여 가설을 검증하고, 그에 따라 자연현상들 사이의 인과관계를 규명하는 수단이다. 따라서 실험은 단순 기능이 아니라, 일련의 숙련된 활동이다. 많은 과학교사들은 '과학은 실천적 학문이기 때문에' 실험을 통하여 과학수업을 해야 한다고 주장한다. 실험 수업은 과학교육이 교육적 위치를 자리 잡아 가는 과정에서 가장 중요한 특징이었고, 이제 실험은 학교 과학에서 확고한 위치를 차지하고 있다. 교사의 효능감은 교사 스스로가 학생의 성취에 영향을 줄 수 있는 능력을 가지고 있다고 믿는 신념 정도를 의미한다. 교육의 실제는 교사 스스로 자신을 어떻게 평가하는지의 사고과정 자체에 더욱 많은 영향을 받는다. 따라서 교수효능감은 교육현장에서 중요한 위치를 차지하고 있으며, 교사의 교수효능감 증진을 교육의 질을 높이는데 우선적으로 실천되어야 할 과제라고 할 수 있다. 본 연구에서는 현직 중등학교 과학교사들의 가지고 있는 실험 관련 인식, 즉 과학과 수업 방법, 과학 수업 및 실험수업지도 능력, 실험수업 빈도, 실험 수업의 장점, 실험 수업의 저해 요인, 실험 수업 목표에 대한 기대 등등에 대하여 조사하고 분석하였다. 이 결과를 통하여 과학실험수업에 대한 실태를 조사하고 효율적인 과학 수업을 위한 방향을 제시하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중등학교에서 이루어지는 경기고사 과학과 지필평가의 실태조사

곽원아, *박현주

*조선대 자연교육대학 *조선대 과학교육학부*

현대 과학교육의 목표인 과학적 소양인은 일상생활의 의사결정에서 과학 지식과 개념을 사용하여 탐구적이고 논리적으로 문제를 해결하고자 한다. 이런 과학교육 목표 달성을 점검할 수 있는 중요한 교육 활동 중의 하나는 학습평가이다. 평가의 목적은 학생들에 대한 다양한 정보와 피드백 자료를 제공 받는 데 있다. 현재 중학교 과학 교과의 내신 평가는 지필평가와 같은 정기고사와 실험보고서, 조사 및 발표를 포함하는 수행 평가로 이루어진다. 그러나 타당도와 신뢰도 측면의 여러 문제점과 한계점에 의해 평가의 대부분은 지필평가로 이루어지고 있다. 이 연구는 현장 과학교사들이 인식하고 있는 중등학교 정기고사 지필평가의 실태를 조사하고 분석하여, 과학교육 평가 분야의 기초 자료로 제공하고자 한다. 연구는 광역시 소재 중등학교에 근무 중인 과학 교사 57 명을 대상으로, 설문지법과 면담법을 병행하여 자료를 수집하였다. 평가 및 평가 목적에 대한 인식, 문항 개발 및 방법, 채점 및 입력 과정, 결과분석 및 피드백, 평가체제의 개선 사항에 대한 의견 등을 조사하여 분석하였다. 분석 결과를 바탕으로 보다 체계적인 평가시스템 도입을 시사점으로 제한하고자 한다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

예비과학(화학) 교사들이 경험한 중등학교 현장에서의 과학 및 화학교육 관련 문제 인식

이금희, *박현주

*조선대 과학교육학과 *조선대 과학교육학부*

이 연구는 교육실습기간 한 달 동안 과학과(화학) 교육실습생들이 인식한 중등학교 현장에서의 과학 및 화학교육 관련 문제를 조사하고 분석하였다. 교육실습생 19 명을 연구참여자로 하여, 교육실습 기간 동안 설문지, 면담, 자기 평가 및 동료 평가, 그리고 지도교사 보고서 자료를 수집하여 분석하였다. 연구참여자들이 교육실습 기간 동안 인식한 교육관련 문제는 학생, 교사, 교육환경, 예비교사와 더불어 교사양성기관으로 나타났다. 예비과학교사들의 과학 교육관련 문제에 대한 인식은 교육 및 교육실습 개선을 위한 시사점을 제공할 것이다.

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

In silico environmental screening for bioconcentraction factor(BCF)

정진희, 차지영, 이성광

한남대 화학과

BCF(bioconcentration factor) is important in the risk assessment of humans and the environment because the chemicals tend to bioconcentrate in aquatic organisms. Therefore, in silico screening is essential for identification and prioritization of new potential bioaccumulative and toxic chemicals.In this study, we have developed in silico models using Quantitative Structure Activity Relationship(QSAR)s for BCF in fish. The experimental BCF data of 685 organic chemicals was collected from high quality BCF database(Arnot and Gobas, 2006) validated by confidence scoring method. 2D chemical structures were transferred to molecular descriptors using PreADMET program. Significant subset of descriptors was selected on the basis of genetic algorithm(GA) combined with support vector machine(SVM), neural network, and multiple linear regression(MLR). Newly designed in silico models could predict the experimental error range of BCF.

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

QSAR modeling for predicting acute toxicity of organic compounds in the rainbow trout (Oncorhynchus mykiss)

송인식, 차지영, 이성광

한남대 화학과

We investigated the acute toxicity in the rainbow trout (Oncorhynchus mykiss), using quantitative structure–activity relationships (QSARs). The models were evaluated on the OECD principles for QSAR validation and the REACH regulatory in the EU. The aquatic toxicity, 96h LC50 (median lethal concentration) of 275 organic pesticides, was obtained from EU-funded project Demetra. Prediction models were derived from 825 molecular descriptors, calculated in PreADMET. Filter methods and a genetic algorithm(GA) were used to select the best subsets of descriptors including cross-validation procedure. Multiple linear regression(MLR), partial least square regression(PLS), artificial neural net(ANN) and support vector machines(SVM) were applied to develop the models fitted for predicting acute toxicity. This models could be useful to reduce the cost of experiments and animals testing.

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

In-situ Preparation of PbS/Polymer Composite Films for Hybrid Solar Cells

곽은주, *우성호, 김화정, 김영규

*경북대 화학공학과 *대구경북과학기술연구원 나노바이오연구부*

Recently hybrid solar cells have gradually come up to the front of next generation solar cells because they could take advantages from both organic and inorganic components. In principle, organic materials could provide easy coating and low-temperature processes, while the stability of devices could be secured by employing inorganic materials. To date, a couple of studies have been reported on the synthesis and application of lead sulfide (PbS) nanoparticles. In most cases, organic ligands were used for delivering better solubility and size uniformity. However, this method has fundamental drawbacks in terms of charge transport owing to the insulating nature of ligand molecules. Hence, in this work, we tried to develop in-situ methods for synthesizing the PbS nanoparticles which are embedded in conjugated polymers. The detailed synthesis and characteristics of PbS/polymer composite films will be presented together with a brief result of hybrid solar cells with them.

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

Hydrogen Storage Behaviors of Chemically Treated Microporous Carbons

이슬이, 박수진

인하대 화학과

In this work, the hydrogen storage behaviors of chemically treated microporous carbon (MCs) synthesized by templating method were investigated. The surface characteristics of the functionalized MCs were confirmed by Fourier transfer infrared spectroscopy and X-ray photoelectron spectroscopy, respectively. The surface functional groups were determined using the Boehm titration method. The hydrogen storage capacity of the MCs was evaluated at 77 K and 1 bar. In the experimental results, it was found that the chemical treatments introduced the oxygen-functional groups onto the MC surfaces. The amount of hydrogen storage was enhanced by acidic surface treatments; meanwhile, the basic surface treatments actually reduced the hydrogen storage capacity of MCs. Consequently, it could be concluded that hydrogen storage behaviors were greatly influenced by the acidic characteristics of MC surfaces, resulting in enhanced electron acceptor-donor interaction at interfaces.

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

Influence of Heat Treatments on Hydrogen Storage Behaviors of Natural Graphite

이슬이, 박수진

인하대 화학과

In this study, heat treatments were performed on natural graphites (NGs) with an acidic gas flow at various temperatures, in an effort to enhance hydrogen storage capacities of the NGs through the modification of NG characteristics. The microstructure and crystallinity of the modified CNTs was evaluated with X-ray diffraction and FT-Raman spectrometer, respectively. The textural properties of the modified NGs were investigated using a nitrogen gas sorption analyzer at 77 K. The hydrogen storage capacities of the modified NGs were investigated by BEL-HP at 77 K/1 bar. From the results, it was found that the heat treatments had influences on the textural characteristics on the modified NGs. Consequently, it was concluded that the heat treatments were major effect to enhance hydrogen storage capacities of NGs.

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

Effect of organic additives on the phase equilibrium of CO2 hydrate

이경진, *이우진

*KAIST *KAIST 건설 및 환경공학과*

We measured the phase equilibrium conditions of CO2 hydrate within the temperature range of 270 – 280K and pressure range of 1.0 – 3.5 MPa. Little change in equilibrium pressure and temperature was observed among the different organic matters. We also evaluated the effect of organic matters on the equilibrium conditions by varying their concentration in the system. The results indicate that organic matters have more shifting effect on the equilibrium conditions when their concentration becomes higher. It is implied that CO2 hydrates formed in natural sediments, which include organic matters with low concentration, can stay stable while CO2 hydrate is developed over a wide range of sediments for CO2 storage.

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

In silico approach for predicting degradation of air persistent organic pollutants(POPs)

차지영, 이성광

한남대 화학과

Atmospheric persistent organic pollutants(POPs) are increasing in a wide range of quantities as large amounts of chemicals have produced annually. Most of air POPs, volatile organic compoundsz(VOCs) caused serious environmental concern are emitted into the troposphere directly and indirectly. The rate constants of reactions between VOCs and oxidants (OH radicals, ozone and NO3 radicals) are one of the most important characteristics related to their degradation in troposphere. In this study, the experimental rate constants of oxidants reactions with 872, 188, 187 organic compounds from literatures were performed in silico approach. Molecular descriptors calculated by PreADMET program were based on 2D chemical structure. The genetic algorithm and the learning methods such as multiple linear regression, artificial neural network were applied to select best subset of molecular descriptors. Final models will give to help identification and prioritization of new potential POPs.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

The role of biopolymers on the kinetics of CO2 hydrate formation for its sequestration

Rheo B. Lamorena, *이우진

*KAIST 건설및환경공학 *KAIST 건설 및 환경공학과*

It has been recognized that gas hydrate formation is influenced by sedimentary inorganic component but little has been paid to the potential influence of sedimentary organic matter. A study was conducted to investigate the effect of biopolymers on the kinetics CO2 hydrate formation. Several water-soluble organic compounds (urea, starch, humic acid) were added into mineral suspensions (marine sediments, kaolinite, Na-montmorillonite, illite, and quartz) and were used as formation media for the hydrate formation tests. Formation media were prepared in both pure deionized water and in electrolyte solutions (3.5% NaCl). Hydrate formation occurred in all formation media without electrolyte within the experimental runtime (

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

Reductive Dechlorination of Terachloroethene by Nano-Sized Zero Valent Iron with Biomimetic Catalyst

amnorzahira, *이우진

*KIST 건설및환경공학과 *KAIST 건설 및 환경공학과*

Catalytic effect of reductive dechlorination of tetrachloroethene (PCE) by nano-sized zero valent iron (nZVI) with biomimetic catalyst (cobalamin (III) and humic acid) was studied in batch reactors. Approximately 90% of PCE was degraded in nZVI/cobalamin(III) suspension, while no significant PCE degradation in nZVI/humic acid suspension at pH 8.2. An estimated kinetic rate constant for PCE dechlorination (0.25 ± 0.01 hr-1) in cobalamin (III)/nZVI suspension was 30 times faster than that in nZVI/humic acid suspension. This is due to formation of cobalamin (II)/cobalamin (III) in nZVI suspension which was identified by spectro-photometric analysis at 405 and 505 nm. 50 - 70% of chloride ion was recovered during the PCE dechlorination. Trichloroethene (TCE) and cis-dichloroethene (cis-DCE) and trans-dichloroethene (trans-DCE) were detected as intermediate products during the reaction. This study provides basic understanding on the function of biomimetic catalyst an electron mediator during the reductive dechlorination of chlorinated organics compound in soil and groundwater.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Effect of TiO_2 size on dye-sensitized solar cells (DSSC)

김승렬, 안호진, *강미숙

*한국과학영재학교 *영남대 화학과*

지난 몇 년 동안 염료감응 태양전지의 핵심 소재인 working 전극으로 사용되는 TiO_2 에 대한 연구가 활발히 진행되고 있다. 본 연구에서는 TiO_2 를 solvothermal processing 에 의해 출발용액의 pH 를 조절하여 세가지 크기의 아나타제 TiO_2 를 합성하여 DSSC 의 scattering material 로 적용하였다. TiO_2 파우더를 합성한 TiO_2 를 용매에 고 분산 시켜 안정한 졸 상태를 만들고 코팅하여 박막을 제조, 건조한 뒤 funace 에 450℃로 소성시켜 0.5 x 0.5(cm2)면적의 단위 셀을 제작하였다. SEM image 를 통하여 입자 크기와 모폴로지를 확인하였으며 그 결과 8.95, 12.79, 20.16 nm 의 세 가지 type 의 크기가 다른 TiO_2 입자를 확인하였고, 이들은 모두 XRD pattern 결과 아나타제의 구조를 나타냈다. solar simulator 로 광효율을 측정한 결과 pH 가 3, 7, 9 로 효율이 6.53, 8.02, 8.61%로 증가함을 확인하였다. 이것은 scattering material 로써 가장 적합한 사이즈는 약 20 nm 임을 말해 주고 있다.

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

Synthesis of P- and B-incorporated TiO2 nanometer sized catalysts for production of hydrogen gas photoelectochemcally

최희찬, 이주승, 안준범, 우재욱, *류시경, **강미숙

*경산과학고 *경산과학고 과학부 **영남대 화학과*

우리나라는 부존자원이 거의 없어 소요에너지의 97%를 수입에 의존하고 있다. 만약, 친환경적이고 경제적인 수소에너지 제조 기술이 개발된다면, 그 기술은 세계 시장에서 큰 경쟁력을 갖게 될 것이다. 따라서 본 연구는 기존의 순수한 TiO2 광촉매와는 다른 새로운 전극 촉매를 개발함에 있어 positive-type 반도체로써 B 이온이, negative-type 반도체로써 P 이온이 함유된 P- 그리고 B-TiO2 나노 광촉매를 합성하여 저급 알코올 분해용 광화학적 수소제조 시스템의 소재로 사용하여 수소를 친환경적이고 효율적으로 생산하는 것을 목적으로 한다. 본 연구에서 개발하고자 하는 나노 소재는 수열합성법의 원리를 도입하여 합성하였다. 합성된 각각의 P(인)- 또는 B(붕소)-TiO2 의 물성을 알아보기 위해 기기분석(XRD, SEM/TEM, UV-visible, Photoluminescence)을 실시하였고, 광화학적 수소제조 시스템을 자체 제작하여 합성한 반도체 소재를 광촉매로 이용하여 저급 알코올(메탄올)을 대상으로 하여 광 전기화적 수소 제조 실험을 실시하였다. 그 결과 B-TiO2 (1mol%)시료가 10 시간 반응했을 경우 수소가 약 0.45ml 발생한 것을 확인 하였다.

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Relationship Between Life Cycle Greengouse Gas Emissions and Life Cycle Cost of Power Generation System

김희태, 김은철, 안태규

성균관대 에너지과학과

All power generation technologies emit greenhouse gases (GHG) and contribute to anthropogenic climate change. It is widely believed that GHG emissions resulting from the use of a particular energy technology need to be quantified over all stages of the technology and its fuel life cycle. Renewable energy including solar PV, wind etc. and nuclear based electricity generation technologies often are deemed to be “carbon free” because their operation do not emit any greenhouse gas. However, it is not that carbon free technology when considering their entire life cycle of electricity generation including power plant construction, operation and maintenance. While accurate calculation of GHG emissions per kilo-Watt-hour (kWh) is often difficult, sound knowledge of life cycle GHG emissions can be an important indicator for mitigation strategies in the power sector. Furthermore, world demand for electricity is expected to grow to about 20,760 TWh in 2015 and to about 28,140 TWh in 2030. Electricity will be play an important role as an essential final energy. At that time, a lot of technologies could generate electricity and the electricity would be considered as a energy product. We need a combined information regarding environmental and economic performance of the various electricity itself to choose preferred power source. In this paper a relative position of each technology on the issue of greenhouse gas (GHG) emissions and cost of electricity generation has been analyzed.

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The change of dye-sensitized solar cells (DSSC) efficiency according to structural difference of TiO_2

안성식, 이현빈, *강미숙

*한국과학영재학교 *영남대 화학과*

태양에너지를 이용한 태양전지의 종류에는 실리콘 태양전지, 무기태양전지, 유기태양전지, 박막태양전지 등이 있다. 이들 중 염료감응 태양전지(DSSC)의 경우 기존의 실리콘 태양전지에 비해 효율은 낮지만 제조단가가 저렴하고 colorful 한 색상을 지니고 있어 각광받고 있다. 이러한 염료감응 태양전지의 구성요소에는 염료, 전해질, TiO2, TCO glass 가 있다. 본 연구에서는 염료감응 태양전지의 구성요소 중 핵심 소재로 주목받고 있는 working 전극으로 사용되는 TiO_2 를 솔-젤법으로 합성한 후 소성온도에 따라 다른 형태의 working 전극으로 사용하여 가장 좋은 효율을 나타내는 구조를 알고자 하였다. 얻어진 TiO_2 Power 를 XRD pattern 으로 확인한 결과 비율이 다른 두 종류의 anatase/rutile 혼합형 rutile 의 두 가지 구조를 확인하였고, SEM image 를 통하여 입자 크기와 모폴로지를 확인하였다. 또한 UV-visible 과 PL 로 흡광도와 발광을 확인하였으며 solar simulator 와 impedance 로 광 효율과 저항을 측정한 결과 rutile 의 비율이 낮은 anatase/rutile 구조에서 4.06%로 가장 우수한 효율을 나타냈다.

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Photocatalytic Hydrogen Production Using Graphite Oxide/TiO_2 Nanocomposite : The Role of Graphite Oxide as an Auxiliary Cocatalyst

박이슬, 최원용

포항공과대 환경공학부

Graphite oxide TiO_2 was prepared by the simultaneous dissociation of bulky graphite oxide and hybridization with TiO_2. Graphite oxide/TiO_2 showed enhanced photocurrent generation and hydrogen production than that of bare TiO_2 under UV light irradiation. The enhanced photocatalytic activity for graphite oxide/TiO_2 was ascribed to the ability of graphite oxide layers in promoting photoinduced charge separation by accepting and transporting electrons from excited TiO_2 to the substrate. Especially, when it coupled with platinum and TiO_2, it shows a synergistic effect for the photocatalytic hydrogen production. It indicates that cheap and abundant carbon conjugated material can be a good candidate for an electron shuttle and an auxiliary co-catalyst for the photocatalytic hydrogen production.

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A novel synthesis of multifunctional iron nano particles using co-solvent system

김재환, 장윤석

포항공과대 환경공학부

Extensive studies for synthesis and characterization of novel nanoparticles with unique reactivity and functions have been made during the recent years. Among the nanoparticles, nanoscale zerovalent iron (nFe) has been used for clinical diagnosis and treatment, as magnetic ferrofluids, in catalysis and as environmental remediants.However, the application of nFe for engineering purposes has several constraints that nFe particles tend to agglomerate and are not easily dispersed in liquids. The agglomeration of nFe can be caused by self assembly of the magnetic nano particles due to their super-paramagnetic property, and the high surface charge with attractive Van der Waals forces. Even if the mechanical agitation process disperses the nFe^{BH} structure in the solution, unstable colloidal property by surface charge of nFe^{BH} particles drives them to agglomerate again. Various efforts have been made to prepare stable nanoscale metal suspensions while maintaining their reactivity via surface modification using surfactants, cellulose and polymers. Although the methods mentioned above (using additives) can partially reduce the aggregation and sedimentation of particles, the development of a method for complete stabilization and dispersion of nFe particles is still necessary because the additives can generate secondary pollution during remediation processes. Here we demonstrated that multifunctional nano iron particles by using co-solvent system can act as efficient nZVI stabilizers for hexavalent chromium (Cr(VI)) removal from water. A possible mechanism for chemical interaction between the synthesized nano particle and Cr(VI) was performed in terms of the structure via sedimentation test, X-ray diffraction (XRD) and transmission electron microscopy(TEM).

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가시광을 흡수하는 염료 감응형 광촉매, TiO_2 섬유 형태와 입자 형태의 수소생산을 통한 광활성 비교 연구

최성규, *김순현, **박현웅

*경북대 물리학과 *대구경북과학기술원 나노바이오연구부 **경북대 물리 및 에너지학부*

지금 까지 TiO_2 광촉매는 큰 밴드갭(3.2eV)을 가지고 있기 때문에 자외선 영역의 빛을 흡수할 수 밖에 없었다. 그러나 자외선은 지표면에 도달하는 태양광에서 단지 1%만이 존재한다. 이에 반해 가시광은 40%정도 존재한다. 보다 높은 태양광의 이용을 위하여 가시광 영역의 빛에서 반응하는 염료를 광촉매에 담지하여 태양광의 효용을 극대화 하는 연구가 진행 중이다. 이러한 목적을 가지고 Eosin Y 염료를 TiO_2 광촉매에 담지하여 물 분해를 통한 수소 생산 효율을 측정 하였다. 우리는 TiO_2 광촉매을 전기방사 과정을 통해 긴 섬유 형태로 만들어 형태의 변화를 통한 입자들과 비교 연구를 시행 하였다. 만들어진 TiO_2 섬유는 500nm 의 직경에 3-4nm 의 mesopores 을 가지며 작은 입자들의 빽빽하게 뭉쳐 있는 구조를 지닌다. 각각의 입자들의 광촉매 비교 실험을 통해 섬유 형태가 입자들 보다 10 배 정도 높은 효율을 확인했다. 작은 입자들이 빽빽하게 뭉쳐져 섬유 형태를 유지 하고 있는 TiO_2 광촉매는 염료에서 들뜬 전자의 전달이 용이하고 전자와 홀의 재 결합을 막아주어 광활성의 증가에 직접적인 원인이 된다. 좋은 광 활성을 가지고 있는 TiO_2 섬유는 친환경에너지로 각광 받고 있는 염료감응형 태양전지에 적용이 가능하다.

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Photoelectrochemical Study on Fe_2O_3-Loaded TiO_2 Nanotubes

전태화, *박현웅

*경북대 에너지협동과정 *경북대 물리 및 에너지학부*

TiO_2 nanotubes (TiNT) have received growing attention due to easy synthesis, unique and robust structure, and relatively high photocatalytic activity as compared to TiO_2 nanoparticles (TiNP). The large bangap (~ 3.2 eV), however, still hinders their wider applications. Various approaches have been made to address the challenge and one of them is to construct hybrid configurations. As an example, this study presents the hybrid of Fe_2O_3 nanoparticles and TiO_2 nanotubes by electrochemically depositing Fe_2O_3 particle in TiO_2 nanotubes grown on Ti foil via anodization. Detailed surface analysis and photoelectrochemical study of Fe_2O_3/TiNT were completed and the results were compared with Fe_2O_3/TiNP.

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Effects of electrolyte and anode composition for electrochemical oxidation of organic

안용윤, *박현웅

*경북대 물리학과 *경북대 물리 및 에너지학부*

Water-treating electrocatalysts have been studied over the four decades and various anodes have been developed and studied. In this study, we have fabricated seven kinds of multi-layered BiOx-doped TiO2 anodes with different coating layers and investigated their electrocatalytic activities for phenol as a model substrate in three different supporting electrolytes (Na2SO4, NaClO4, and NaCl). It has been found that the activity was significantly affected by the compositions of outmost layer and also supporting electrolytes. More detailed experimental results on surface analyses (XRD, XPS, SEM, etc), degradation kinetics of phenol along with CO2 generation, and simultaneous hydrogen production from water will be presented.

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TiO2 films made from N3-dyed TiO2 dispersions for DSSCs adaptable to a low-temperature continuous printing process

표명호, *김현호

*순천대 화학과 *순천대*

For the fabrication of dye-sensitized solar cells (DSSCs) through a continuous printing process, photoanode films are prepared using N3-dyed TiO2 nanoparticle (N3/TiO2) dispersions rather than by adsorbing N3 dyes onto TiO2 films (TiO2-N3). No high temperature sintering for TiO2 is involved. Instead, inter-particle connections are induced by pressurization. Investigation of the photovoltaic performance of DSSCs composed of pressurized N3/TiO2 reveals that pressurized N3/TiO2 with moderate dye-loadings produces a power conversion efficiency (h) that is comparable to pressurized TiO2-N3 and a higher h than N3-adsorption onto pressurized TiO2 (PTiO2-N3). Despite a decreased recombination process, high dye–loading of N3/TiO2 results in a decrease in the h′ due to insufficient inter-particle connection. The application of 10 ~ 35 MPa to N3/TiO2 is sufficient, as a greater pressure leads to a negligible decrease of the electron transport resistance through TiO2. The optimal film thickness after pressurization is ca. 6.0 mm, which is quite thinner than the film thickness showing the best performance in DSSC produced by the high-temperature sintering of TiO2. The best photovoltaic performance of DSSCs composed of N3/TiO2 (dye-loading = 9.0 x 10-11 mol cm-2) pressurized at 34 MPa is a h of 5.3 %, a short circuit current density (Jsc) of 9.2 mA cm-2, an open circuit voltage (Voc) of 775 mV, and a fill factor (FF) of 74 %.

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Distinction of domestic products by organochlorine pesticide (OCP) profiles in tea

손민희, 장윤석

포항공과대 환경공학부

The four kinds of tea samples were analyzed to investigate the profiles of 22 organochlorine pesticide (OCP) according to their origin. The abundant contaminants detected were α-hexachlorohexane(HCH), hexachlorobenzene(HCB), and DDT, however, the other OCPs including aldrin, dieldrin, and endrin were not detected in all tea samples. These results suggested that it was possible to distinguish between domestic and imported goods by the profiles of featured compounds such as DDT and mirex. Although most of countries have banned and restricted the use of OCPs, much amount of OCPs still remained in the environment due to their physico-chemical characteristics such as persistency, long-range transport, and bioaccumulation.

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Dietary intakes of polychlorinated biphenyls in Korea

손민희, 장윤석

포항공과대 환경공학부

We developed an isotope dilution method for total polychlorinated biphenyls (PCBs) included 7 indicator congeners, which was applied to retailed foods. 5 different market baskets consisting of almost 210 individual food samples representing 42 different food items were analyzed to estimate daily PCB intakes based on food intake(g/day) published Ministry for Health, Welfare and Family Affairs and mean body weight (55 kg) of Korean.

THE KOREAN CHEMICAL SOCIETY

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Simultaneous Acceleration of Cr(VI) and As(III) Removal by Freezing

김기태, 최원용

포항공과대 환경공학부

The redox transformation of trace elements (chromium and arsenic) controls the bioavailability, mobility, toxicity, and their environmental fate. Therefore, investigations on the reactions of chromium and arsenic at environmental interfaces are very crucial for predicting and preserving environmental health and enable to provide new inspirations for remediation strategies. In this work, the simultaneous redox reactions between Cr(VI) and As(III) in polycrystalline ice were investigated under various conditions. The Cr(VI) reduction with As(III) proceeded negligible rate in aqueous solution was significantly accelerated in ice phase regardless of different initial concentration of Cr(VI) and increased with increasing the added As(III) concentration. Interestingly, Cr(VI) reduction and As(III) oxidation was markedly accelerated in all ranges of pH (pH 2 - 11) tested in polycrystalline ice phase whereas the Cr(VI)/As(III) removal by redox processes in aqueous solution were negligible. The Cr(VI) reduction and As(III) oxidation in ice phase seems to proceed stoichiometrically in all pH ranges. The enhanced Cr(VI)/As(III) removal by freezing is explained by enriched As(III) molecules as reductant and lowered pH value in ice crystal grain boundaries, that is “freeze concentration ” and “pH change” respectively. Our results imply that the intrinsic transformation by freezing can provide a new pathway or possibility of natural detoxification of chromium and arsenic in cold environment such as in upper troposphere, high latitudes(including polar regions) or mid-latitudes during winter season and apply to new engineered remediation strategies for Cr(VI) and As(III) removal.

대한화학회 제106회 총회 및 학술발표회 (The 106th National Meeting of the Korean Chemical Society)

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The redox transformation of trace elements (chromium and arsenic) controls the bioavailability, mobility, toxicity, and their environmental fate. Therefore, investigations on the reactions of chromium and arsenic at environmental interfaces are very crucial for predicting and preserving environmental health and enable to provide new inspirations for remediation strategies. In this work, the simultaneous redox reactions between Cr(VI) and As(III) in polycrystalline ice were investigated under various conditions. The Cr(VI) reduction with As(III) proceeded negligible rate in aqueous solution was significantly accelerated in ice phase regardless of different initial concentration of Cr(VI) and increased with increasing the added As(III) concentration. Interestingly, Cr(VI) reduction and As(III) oxidation was markedly accelerated in all ranges of pH (pH 2 - 11) tested in polycrystalline ice phase whereas the Cr(VI)/As(III) removal by redox processes in aqueous solution were negligible. The Cr(VI) reduction and As(III) oxidation in ice phase seems to proceed stoichiometrically in all pH ranges. The enhanced Cr(VI)/As(III) removal by freezing is explained by enriched As(III) molecules as reductant and lowered pH value in ice crystal grain boundaries, that is “freeze concentration ” and “pH change” respectively. Our results imply that the intrinsic transformation by freezing can provide a new pathway or possibility of natural detoxification of chromium and arsenic in cold environment such as in upper troposphere, high latitudes(including polar regions) or mid-latitudes during winter season and apply to new engineered remediation strategies for Cr(VI) and As(III) removal.