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Hydrogen Production from Methanol Photolysis in Aqueous Solution Using Bimetallic Zinc Indium Sulfide Catalysts

Misook Kang*, Suhwan Choi and Jeong Yeon Do

Department of Chemistry, College of Natural Sciences, Yeungnam University, Gyeongsan, Gyeongbuk, South Korea

Abstract

Water or light alcohols decompositions through the photochemical reaction for hydrogen production are advantageous in that the reaction can proceed using only the sunlight without any additional energy. However, there is required at least 0.7-1.2 eV of voltage to photolysis of water or light alcohols. Therefore, semiconductor materials such as TiO_2 containing a band-gap exceeding this voltage and redox potential ranges for hydrogen and oxygen are need. In recent years, many researchers attention shifted to some semiconductors absorbing visible light, and more attention was focused on semiconductors with sulfur counter ions from oxygen.

This study focuses on hydrogen production by methanol photolysis using zinc indium sulfide. The X-ray diffraction peaks which assigned to hexagonal $\text{Zn}_3\text{In}_2\text{S}_6$ structure are shown in the synthesized $\text{Zn}_2\text{InS}_{2.5}$ and $\text{ZnInS}_{2.5}$ samples, however, a perfect hexagonal ZnIn_2S_4 structure is observed when In of twice amount against Zn is coexisted. The results of ultra-violet absorption and X-ray photoelectron spectroscopy-edge analysis confirm that the band-gaps of $\text{Zn}_x\text{In}_y\text{S}_z$ particles decrease depend on the coexistence of In. However, the photocurrent which related to the life time of excited electrons is no correlation with the Zn/In molar ratio, and it is higher in $\text{ZnInS}_{2.5}$ particle with a ratio of Zn:In=1:1. Consequently, the hydrogen production by methanol decomposition in aqueous solution is the best in $\text{ZnInS}_{2.5}$ catalyst. This result gives ultimately relevant that the recombination between electrons and holes during photocatalytic methanol decomposition is suppressed over bimetallic $\text{ZnInS}_{2.5}$ than pure single metallic ZnS.

Ion Beam Sputter Deposition Technique for Direct Growth of Ge Quantum Dots on a Graphene/ SiO_2 /Si Substrate

Yu Yang^{1,2*}, Tao Sun^{1,2}, Tianjian Zeng¹, Zhang Zhang¹ and Chong Wang^{1,2}

¹*School of Energy, Yunnan University, China*

²*Institute of Optoelectronic Information Material, School of Materials Science and Engineering, Yunnan University, China*

Abstract

The quantum dots (QDs)/graphene hybrid structure shows excellent photoresponse abilities in photodeficiency devices due to the unique QDs quantum confinement and the ultrahigh carrier mobility of graphene. Thus, this project invented the ion beam sputtering deposition technique (IBSD) to realize the directly growth of Ge quantum dots (QDs) on single-layer graphene on a SiO_2 /Si substrate.

The morphology results illustrate that the Ge QDs size and morphology on graphene can be modulated via tuning the Ge coverage by IBSD technique. The results also indicate that increasing the sputtering time of Ge, the density of Ge dots increased, but the sizes (both diameter and height) of Ge dots tend to decrease. All morphology evolution route of Ge islands agrees well with the Zinsmeister theory. Secondly, the existence of interaction like doping effects at the interface of Ge QDs with graphene has been demonstrated. The strength of the interaction can be enhanced remarkably by reducing the Ge coverage in a certain scope, which indicates that the interaction can be modulated via controlling the coverage of Ge. The charge transfer behaviour at the interface of Ge/graphene has been demonstrated also. Comparing with traditional methods for Ge dots grown on Si substrate, the IBSD treatment changes the positions of corresponding photoluminescence (PL) peaks of Ge QDs/graphene hybrid structure undergo a large red-shift, which was attributed to the lack of atomic intermixing and the existence

of surface states in this hybrid material. According to the first principle calculation, the Ge growth on the graphene follows the Volmer–Weber mode instead of the traditional Ge QDs/Si system Stranski–Krastanow mode. The theoretical study also suggests that decreasing the Ge coverage enhances the interaction between Ge and graphene layer, which highly agree with the experimental results.

The final products were applied in a FET photodetectors, the device demonstrates the responsivity of 4.3 AW-1 at 808 nm infrared light irradiation and relatively large values (0.92) of β in absolute. The optoelectronic features indicate that the device using IBSD fabricated Ge QDs/graphene improves the efficiency of carrier transfer and overcome the limit of ligand barrier at the interface of Ge/graphene. This project supplies a new technique for fabricating hybrid nanostructure QDs/graphene for novel optoelectronic devices application.

Charge Transport, Interfacial Interactions and Synergistic Mechanism in BiNbO₄/MWO₄ (M = Zn and Cd) Heterostructures for Hydrogen Production: Insights from a DFT+U Study

Francis Opoku¹, Krishna Kuben Govender², Cornelia Gertina Catharina Elizabeth van Sittert³ and Penny Poomani Govender^{1*}

¹Department of Applied Chemistry, University of Johannesburg, Doornfontein Campus, Johannesburg, South Africa

²Council for Scientific and Industrial Research, Meraka Institute, Center for High Performance Computing, Cape Town, South Africa

³Research Focus Area for Chemical Resource Beneficiation: Laboratory of Applied Molecular Modelling, North-West University, Potchefstroom, South Africa

Abstract

In the 21st century, the growing demand of global energy is one of the key challenges. The photocatalytic generation of hydrogen has attracted extensive attention to discuss the increasing global demand for sustainable and clean energy. However, hydrogen evolution reaction normally uses the economically expensive rare noble metals and the process remains a challenge. Herein, low-cost BiNbO₄/MWO₄(010) heterostructures are studied for the first time to check their suitability towards photocatalytic hydrogen production. A theoretical study with the aid of density functional theory (DFT) is used to investigate the synergistic effect, ionisation energy, electron affinity, charge transfer, electronic properties and the underlying mechanism for hydrogen generation of BiNbO₄/MWO₄(010) heterostructures. The experimental band gaps of bulk ZnWO₄, CdWO₄ and BiNbO₄ are well reproduced by the DFT+U method. The calculated band edge position shows a type-II staggered band alignment and the charge transfer between BiNbO₄ and MWO₄ monolayers results in a large interfacial built-in potential, which will favour the separation of charge carriers in the heterostructures. The effective mass of the photoinduced holes is higher compared to the electrons, making the heterostructures useful in hydrogen production. The BiNbO₄/MWO₄(010) heterostructures are more suitable for photocatalytic hydrogen production due to its strong reducing power relative to the H⁺/H₂O potential. This study sheds insight on the less known BiNbO₄/ZnWO₄(010) heterostructures and the fully explored electronic and optical properties will pave way for future photocatalytic water splitting applications.

The Magnetic and Electrocatalytic Properties for Ni_xPt_{1-x} Nanoalloys

Aixian Shan^{1*} and Chinpeng Chen²

¹School of Mathematics and Physics, University of Science and Technology Beijing, Beijing, China

²Department of Physics, Peking University, Beijing, China

Abstract

We have synthesized bimetallic NiPt₂ nanoalloys via a simple one-pot wet chemical method. They are sub-7 nm monodispersed single-crystal with the morphology of truncated octahedrons in the alloying state of disordered atomic arrangements. The effective magnetic moments exhibit two unusual properties. Firstly, an anomalous temperature dependency is observed, increasing from approximately 0.9 μ B/atom at 15 K to 1.9 μ B/atom at 300 K. Secondly, the magnitude of the average effective moment for the Ni atoms increases by a factor of more than three compared with bulk counterpart at room temperature. To understand these intriguing properties, we have carried out experiments by X-ray absorption near-edge spectroscopy (XANES) of the L3 edge for Pt and numerical calculations by density functional theory. The observed novel enhancement in magnetism and its anomalous temperature dependency are attributable to the electron transfer arising from the thermal-activation effects. The electron transfer might play important roles in the material functionalities not only for magnetic but also for electrocatalytic properties. To investigate the electrocatalytic properties, we have also synthesized Ni_xPt_{1-x} nanoalloys with controllable shape, size and compositions. Their electrocatalytic properties for the oxidation of methanol are apparently better than that the commercial Pt/C catalyst. This makes the Ni_xPt_{1-x} nanoalloys potential candidates as fuel cell catalysts.

Preparation of Ge Quantum Dots on Graphene/SiO₂/Si Substrates by Sputtering Deposition

Anran Chen^{1,2*}, Jin Zhang^{1,2} and Yu Yang^{1,2}

¹School of Energy, Yunnan University, China

²Institute of Optoelectronic Information Material, School of Materials Science and Engineering, Yunnan University, China

Abstract

Graphene-based hybrid materials combined with nanometer materials has gained a great research interests due to its novel promising applications. Here, we fabricate a composite of Ge Quantum dots (QDs) grown on graphene/SiO₂/Si substrate by self-assembled ion beam sputtering deposition (IBSD) technique with growth interrupt. All the samples were grown under 500 °C and the interrupt time was all set as 10 minutes with different deposition time. The evolution behavior and the doping effect were investigated by atomic force microscope (AFM) and Raman spectra. The size and density of Ge QDs increase first and then decrease with the increase of deposition time. When deposition time is 180 s, the density of Ge QDs can reach to 109/cm², and its morphology and size are the most uniform. At the same time, Red shift of G peak in Raman spectra indicates charge doping effect between Ge and graphene. Our research provides preliminary study for preparation of Ge QDs/graphene composites and use for optoelectronic devices to improve photoelectric properties.

Synthesis of Molybdenum Sulphide Nanostructures for the Treatment of Pollutants in Water

Leelakrishna Reddy* and Madima Ntakadzeni

Department of Applied Physics and Engineering Mathematics, University of Johannesburg, Doornfontein Campus, South Africa

Abstract

Water pollution is a major hazard for humankind; the subsequent effect is the scarcity of clean drinking water. These effects are experienced both in South Africa and in the world at large, thus the demand for clean drinking water has posed a challenge for researchers. The commonly found pollutants in water are the dyes Methyl Blue (MB) and Rhodamine (RhB) as well as the heavy metals, such as Chromium (VI). These are found to be the major contributors to pollution in water. The aim of this research is to fabricate nanostructured compounds for the removal of these dyes and heavy metals from water. In this regard, molybdenum sulphide and its nanostructure composites are synthesized to evaluate its photocatalytic properties with respect to water treatment. Molybdenum sulphide nanostructures are synthesized via hydrothermal methods using various capping agents, such as Polyethylene glycol (PEG-400) and Ethylenediaminetetraacetic acid (EDTA) as the samples PEG-MoS₂ and EDTA-MoS₂ respectively. Further, the nanocomposites of EDTA-MoS₂ and manganese chloride are also synthesized for the removal of chromium. Results show that by using PEG-MoS₂, a degradation efficiency of 97.3% for RhB is achieved in a time of 75 minutes, while a 98.1% efficiency of MB removal is achieved in a time of 90 minutes. On the other hand, the use of EDTA-MoS₂ for the removal of the dyes RhB and MB are found to be 86.5 and 99.8%, respectively efficient in a time interval of 90 minutes. Likewise, the PEG-MoS₂ nanostructures are tested for the catalytic reduction of chromium and are found to have an efficiency of 91.1% in a time interval of 75 minutes.

Route of Preparation a High Surface Area Zirconium Oxide

Rudzani Sigwadi^{1*}, Mokhotjwa Dhlamini², Touhami Mokrani¹ and Fulufhelo Nemavhola³

¹Department of Chemical Engineering, University of South Africa, South Africa

²Department of Physics, University of South Africa, South Africa

³Department of Mechanical and Industrial Engineering, University of South Africa, South Africa

Abstract

Stable and high-surface-area zirconia oxide nanoparticles have been synthesized by means of the hydrothermal method. The BET results show a high surface area of 543 m²/g was obtained in the hydrothermal process, having a high porosity in nanometer range. The hydrothermal method was operated at 120 °C, under autoclave with a Teflon liner at ambient pressure for 48 hours. High resolution Scanning Electron Microscopy (HRSEM) shows the different morphologies of zirconia nanoparticles, which could be categorized as one-dimensional (1D) and zero-dimensional (0D), as it had a high crystallite orientation, which was also confirmed by the X-ray diffraction (XRD). The mixture of two types of cubic phase in one sample was obtained from XRD and confirmed by the zirconium nanostructure, which shows the stable phase of fluorite, which has full cubic symmetry (Im-3m) and also an Arkelite zirconia nanostructure that shows the stable phase of fluorite, which has full cubic symmetry (Fm-3m). The XRD results also shows the different structure orientations of face-centered cubic (FCC) and body-centered cubic (BCC) in one sample.

Bonding Strength of Vertically Aligned CNTs Grown on Cu Substrates: Effect of Buffer Layer

QiuHong Zhang^{1*} and Levi Elston²

¹University of Dayton Research Institute (UDRI), Dayton, OH, USA

²Air Force Research Laboratory (AFRL), WPAFB, OH, USA

Abstract

Direct growth of vertical aligned carbon nanotubes (VACNTs) onto bulk copper (Cu) substrates is a promising application of utilizing CNTs as novel thermal interface materials (TIMs) for electronics packaging. The previous study's results demonstrated that buffer layer plays a key role in the growth of CNTs on Cu structure, and by introducing appropriate controlled buffer layers, VACNTs with good alignment and high quality can be synthesized reproducibly on Cu substrates via chemical vapor deposition. However, one of the more fundamental issues, effect of buffer layer on CNT/Cu interfacial property, especially on bonding attachment strength, is not fully understood. In the present study, the effect of buffer layer, including materials (Al_2O_3 , SiO_2 and Al), thickness and deposition method, on CNT/Cu interfacial bonding strength was investigated using a uniaxial force testing system. The interface morphology of CNT/Cu substrates after pull-off testing was characterized using SEM. The experimental results indicated that buffer layer not only dictated CNT/Cu substrate bonding strength, but also affects CNT/Cu fracture location and interface morphology. This quantitative evaluation and fundamental understanding of the effect of buffer layer on CNT/Cu substrate interface bonding strength would ultimately lead to development of well-bonded VACNT nanostructured devices for a real-life electronics applications.

Mechanical Properties of BN Nanosheets

Alexey Falin^{*}, Ying Chen and Luhua Li

Deakin University, Australia

Abstract

With occurrence of graphene in 2004, two-dimensional (2D) materials have received significant interest from both academic and industrial communities. The non-carbon 2D nanosheets, such as boron nitride (BN), molybdenum disulfide (MoS_2) also attracted a lot of attention due to their unique physical properties. In spite of extensive studies on the properties of 2D materials, the mechanical properties of various nanosheets and factors affecting them have not been studied experimentally. These properties have considerable importance not only from the fundamental point of view but also for future applications of nanosheets.

This work is a short review of the mechanical properties of BN nanosheets. It has been shown that Young's modulus and fracture strength of monolayer (1L) BN are close to those of graphene. However, with the increasing number of the layers, the mechanical properties of graphene started to deteriorate up to 30% while BN nanosheets were as strong as 1L BN. According to the theoretical calculations, the interlayer interaction in BN increased with increasing in-plane strain and out-of-plane compression. The interlayer interaction in graphene at the same conditions decreased which led to the interlayer slide. Also, the mechanical properties of nanosheets were highly influenced by defects and temperature.

The study of mechanical properties of BN nanosheets showed their high potential to substitute graphene nanosheets in various application almost without sacrificing the required strength and stiffness. The high-temperature stability of BN nanosheets also can be used for composite production in the areas where graphene fillers may cause rapid oxidation at elevated temperatures.

Role of MoS_2 and WS_2 Monolayers on Photocatalytic Hydrogen Production and the Pollutant Degradation of Monoclinic BiVO_4 : A First-principles Study

Francis Opoku^{1*}, Krishna Kuben Govender², Cornelia Gertina Catharina Elizabeth van Sittert³ and Penny Poomani Govender¹

¹Department of Applied Chemistry, University of Johannesburg, Doornfontein Campus, Johannesburg, South Africa

²Council for Scientific and Industrial Research, Meraka Institute, Center for High Performance Computing, Cape Town, South Africa

³Research Focus Area for Chemical Resource Beneficiation: Laboratory of Applied Molecular Modelling, North-West University, Potchefstroom, South Africa

Abstract

The global dependence on exhaustible fossil fuel resources has made the search for an alternative renewable and sustainable

fuel more urgent. Fabricated m-BiVO₄-based heterostructures have shown improved photocatalytic activity for hydrogen evolution and pollutant degradation; however, a deeper understanding of the photocatalytic mechanism and the role of the monolayers is still lacking. In the present study, the roles of MoS₂ and WS₂ monolayers loaded onto an m-BiVO₄ surface for active photocatalytic hydrogen production and pollutant degradation are explored using first-principle studies. Herein, hybrid density functional calculations are used to investigate the charge transfer, electronic properties, photocatalytic activity and mechanism of the MS₂/m-BiVO₄(010) heterostructures. The results showed a narrow band gap, built-in potential and a type-II band alignment for the MS₂/m-BiVO₄(010) heterostructures compared to pure m-BiVO₄, which favor the separation and transfer of charge carriers and visible-light-driven activity. The MoS₂/m-BiVO₄ heterostructure showed a suitable band edge for hydrogen production and pollutant degradation compared to the WS₂/m-BiVO₄ heterostructure. This improvement is attributed to the role of the MoS₂ monolayer as an electron donor, the many reactive sites on the MoS₂ surface and the enhanced electron/hole pair separation of charge carriers at the MoS₂/m-BiVO₄(010) interface. Based on the analysis of the electronic properties, the MS₂/m-BiVO₄(010) heterostructures are shown to fit within the acceptable band gap and built-in potential range. The proposed theoretical design paves a way for the effective and large-scale fabrication of m-BiVO₄-based photocatalyst for solar energy conversion and environmental remediation applications.

Synthesis of Hollow-structured Metal Oxide Nanomaterials Formed from Nanostructured Metal Chalcogenide and their Application to Lithium Ion Battery

Gi Dae Park* and Yun Chan Kang

Department of Materials Science and Engineering, Korea University, Anam-Dong, Seongbuk-Gu Seoul, South Korea

Abstract

Hollow-structured nanomaterials with various morphologies, including nanospheres, nanoplates, and nanorods, have attracted significant attention because of their widespread applications in energy storage, catalysis, drug delivery, and gas sensors. In particular, when it is applied as anode materials for lithium-ion batteries, the large portion of void space in hollow-structured nanomaterials has been used to accommodate large volume changes during cycling, to provide short path length for lithium-ion transport. Hollow-structured nanospheres have been widely synthesized by various method with use of template. However, templates with 1D or 2D structured nanorod and nanoplate have not been well developed. Therefore, hollow-structured 1D and 2D nanomaterials were prepared via the Kirkendall effect without the use of templates. In recent, hollow structured 1D and 2D metal chalcogenides have been reported by using 1D and 2D structured metal oxide nanomaterials via the Kirkendall effect. However, metal chalcogenides materials rarely transformed into their metal oxide materials with unique morphology. In this study, the transformation of nanostructured metal sulfides and selenides into uniquely structured metal oxides via the Kirkendall effect is studied. Hollow SnO₂ nanoplate and hierarchically structured SnO₂ microspheres comprising hollow SnO₂ nanoplate are synthesized by spray pyrolysis applying a Kirkendall diffusion process. The uniquely structured metal oxide hollow nanoplates have extremely superior cycling and rate performances for Li-ion storage.

Presence of Valence Sulfide and Oxide Impurities in MoS₂ and WS₂ can Dramatically Change their Hydrogen Evolution Reaction Activities

Naziah Mohamad Latiff¹, Lu Wang¹, Carmen C. Mayorga-Martinez¹, Zdeněk Sofer², Adrian C. Fisher³ and Martin Pumera¹

¹Nanyang Technological University, Singapore

²University of Chemistry and Technology Prague, Czech Republic

³University of Cambridge, UK

Abstract

Hydrogen evolution reaction (HER) is important for the clean production of hydrogen gas for a hydrogen economy. Currently, platinum is known to be the best HER electrocatalyst. However, its high price and limited abundance impedes the progress of this technology. This has motivated an intensive search for alternative HER electrocatalysts. Molybdenum disulfide (MoS₂) and tungsten disulfide (WS₂) are touted as promising future replacements of platinum in electrolyzers. However, there is significant discrepancy in the HER onset potentials of MoS₂ and WS₂ reported. In this paper, we show that the presence of their valence sulfide and oxide impurities namely MoS₃, MoO₂, MoO₃, WS₃, WO₂ and WO₃ can contribute to the HER performances of MoS₂ and WS₂.

PtTe₂ as a Safe Alternative Electrocatalyst for Oxygen Reduction Reaction (ORR)

Nur Farhanah Binte Rosli^{1*}, Carmen C. Mayorga-Martinez¹, Naziah M. Latiff¹, Nasuha Rohaizad¹, Zdeněk Sofer², Adrian C. Fisher³ and Martin Pumera¹

¹Nanyang Technological University, Singapore

²University of Chemistry and Technology Prague Technická, Czech Republic

³University of Cambridge, UK

Abstract

Oxygen reduction reaction (ORR) is an important reaction for fuel cells. Platinum on carbon (Pt/C) is a typical electrocatalyst for ORR in industrial applications. There is a constant search for a replacement for Pt/C with better ORR electrocatalytic performance but thus far, most materials show poorer electrocatalytic activity than Pt/C. Herein, we present electrocatalytic and cytotoxicity studies of platinum (Pt) dichalcogenides and we have found PtTe₂ to have similar electrocatalytic ORR performance to Pt/C but with significantly lower toxicity. Hence, PtTe₂ can be denoted as a safer alternative electrocatalyst for ORR. In summary, these studies can allow better understanding of electrocatalytic performance and toxicological profiles and of Pt dichalcogenides in comparison to Pt/C to aid future mass application and commercialisation in clean energy reactions such as ORR.

The Influence of Spin Speed Effect on ZnO Seed Layers on ZnO Nanorods-based Perovskite Solar Cells

Wei-Shuo Li¹, Yun-Hao Chen and Huang-Chung Cheng

Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan

Abstract

Perovskite solar cells have drawn significant attention due to the outstanding efficiency and low-cost fabrication process. In this study, ZnO nanorods is chosen as the electron transport layer (ETL) due to its 3D structure and low temperature process. While depositing perovskite layer, we used two-step coating method to improve the surface coverage and the uniformity of the perovskite layer. To further improve the performance of the solar cells, we tune the spin speed of the ZnO seed layer which can control the density of ZnO nanorods. The power conversion efficiency of 9.50 % is achieved with the spin speed of 4500 rpm.

Synthesis and Application of a Sustainable N-doped TiO₂/CdS Nanohybrid Composite for Photocatalytic Degradation of 4-chlorophenol

Alexander G. Aragon^{1*}, Wallace Kierulf-Vieira¹, Tomasz Łęcki², Magdalena Skompska² and Justyna Widera-Kalinowska¹

¹Department of Chemistry, Adelphi University, NY, USA

²Faculty of Chemistry, University of Warsaw, Poland

Abstract

Titanium dioxide (TiO₂), a semiconducting metal oxide, has gained much attention for its potential application as a photocatalyst over the past few decades. However, TiO₂ is characterized by a wide optical bandgap (E_g~3.2 eV) that requires UV irradiation, leading to limited visible solar light application [1]. Doping with nitrogen and combining with a narrow bandgap semiconductor such as CdS (E_g~2.48 eV) has the potential to resolve these issues [2]. CdS, however, undergoes photocorrosion with photogenerated holes. Hole scavengers, such as S²⁻ ions, may suppress this process. In this work, we propose an alternative approach involving the protection of CdS deposited on TiO₂ with a thin film of conducting polymer. Nitrogen-doped TiO₂ (N-TiO₂) nanostructures were synthesized on FTO glass using a sol-gel method. Sequentially, CdS nanoparticles were deposited via SILAR, and poly(1,8-diaminocarbazole) (PDACz) [3] was synthesized on their surface to form the full hybrid photocatalyst. The bandgap energy of the N-TiO₂/CdS/PDACz hybrid determined from UV-Vis reflectance spectra was 2.26 eV, close to that of CdS. The synthesized TiO₂ nanostructures, along with N-TiO₂, N-TiO₂/CdS and N-TiO₂/CdS/PDACz composites were applied to visible light photodegradation of 4-chlorophenol. The N-TiO₂/CdS system yielded the highest photocatalytic reaction rate (k = 0.00360 min⁻¹) compared to bare TiO₂ (k = 0.00140 min⁻¹). Despite this, significant photocorrosion of CdS was confirmed by UV-Vis reflectance spectra taken post-photocatalytic measurement. The N-TiO₂/CdS/PDACz hybrid showed a middle value of photocatalytic rate constant (k = 0.00201 min⁻¹) and dissolution of CdS was significantly inhibited by the presence of the polymer, making this system attractive for practical applications.

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Comparative Study of H₂ Adsorption on Na Doped SiC and SiGe Monolayers

L.G. Arellano¹, F. de Santiago¹, A. Miranda¹, L.A. Pérez² and M. Cruz-Irisson¹

¹Instituto Politécnico Nacional, ESIME-Culhuacán, Ciudad de México, México

²Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México, México

Abstract

The silicon carbide monolayer (SiC-M) has recently attracted considerable attention due to its outstanding properties such as high mechanical strength, saturated carrier mobility, high thermal stability, and high thermal conductivity. Compared with graphene, SiC-M has a much higher chemical reactivity towards foreign adsorbates, rendering it a potential metal-free catalyst. The siligene monolayer (SiGe-M) is stable and free from imaginary frequency in the phonon spectrum. The Ge and Si atoms in SiGe-M exhibit different tendencies in binding with hydrogen atoms, making sublattice-selective hydrogenation and consequently electron spin-polarization possible. The SiC-M and SiGe-M with metal atoms have been recognized as promising materials for the storage of hydrogen. In the present study we report the molecular c SiGe-M both doped with Na. The calculations have been performed density functional theory. For the SiC-M, the Na adsorption favors the “top” site, conversely, the SiGe-M favors the “hollow” site. The interaction of the Na-doped monolayers with molecular hydrogen suggests that each Na atom can bind up to four hydrogen molecules with average adsorption energy of 0.79 eV for the SiC-M, and of 0.25 eV for the SiGe-M. All these observations suggest that a large storage capacity can be obtained for the SiC-M and SiGe-M. Then, these materials can be considered for the storage of hydrogen.

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Green Solar Cell

Dev R. Udata

Valley Catholic School, Beaverton, OR, USA

Abstract

Solar cells convert sunlight into electrical energy, and they have a large role to play in boosting solar power generation globally. But the cost of solar power is still high and not everyone can afford it in many parts of the world. Currently, materials used to make solar cells are environmentally harmful and toxic to human beings. To overcome the above challenges, I have developed a type of solar cell that can convert a wide range of sunlight into usable electrical energy at very low cost and also with environmentally safe materials.

This green solar cell design and principle mimics the natural photosynthesis in plants and produces electricity through electron transfer. When the sunlight hits the conductive glass with the plant extract it absorbs the sunlight there. With the help of the carbon layered slide and electrolyte solution it will produce current.

I used numerous combinations of natural plant materials such as raspberry, blueberry, blackberry, grapes, spinach, henna, and cilantro to find out efficient natural material which can take up light and excite the electrons to produce electricity over the period of 15 days. The plant extract of spinach produced the most current out of all the natural plant extracts.

To further improve cost efficiency and better performance of solar cells in a greener way, I would like to explore more natural materials to substitute to Titanium Dioxide. Also, would like explore alternative natural materials like cuticle, plant wax etc. to replace anti-reflective glass.

Utilizing Quantum Key Distribution within Nanotechnology

Gretchen Farrow^{*} and Danny Barnes

Department of Computer Science, School of Science, Hampton University, Hampton, VA, USA

Abstract

New technologies are emerging yearly with every enhancement. With technology getting faster and smaller, security is needed at a much higher rate due to privacy issues. Nanoscience and nanotechnology are both the now and the future. Nanotechnology can be the vanguard of innovations for security. Often times, security has the lowest priority when implementing new ideas. This lack of thought could cause a host of vulnerabilities in the implementation, thus creating a negative stigma for the technology. Quantum Key Distribution is a method of using quantum states to establish a random secret key for encryption and is a subset of Quantum Computing. Quantum Key Distribution promises unconditional security in data communication and is currently being placed in commercial applications. Nanotechnology is evolving and creating the need to evolve Quantum Key Distribution. This research will utilize online quantum computer simulators to implement common Quantum Key Distribution protocols. Furthermore, this research will investigate the possibility of quantum computing systems being transferred to nanoscience/nanotechnology. Also, the research will include how quantum computing can enhance the security of nanotechnologies without hindering the capabilities.

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Characterization of CuS@CuInS₂:In₂S₃ Particles for Effective Hydrogen Production from Water/Methanol Photo Spitting

Jeong Yeon Do^{*} and Misook Kang

Department of Chemistry, College of Natural Sciences, Yeungnam University, Gyeongsan, Gyeongbuk, South Korea

Abstract

Since industrialization, humanity faces environmental pollution and energy depletion, and hydrogen energy is attracting attention as a next-generation clean energy resource that can solve this problem. The most environmentally friendly and economical way to produce hydrogen is through the use of photocatalysts, and it is essential to develop highly efficient photocatalysts. Titanium dioxide (TiO₂), which is a typical photocatalyst, has various advantages such as low cost, high oxidation potential and non-toxicity, but has little optical activity in the visible region and is difficult to commercialize due to high recombination rate of photo-generated charge carriers. Accordingly, a sulfide catalyst, which is effective for charge separation and excellent in response in the visible light region, has recently been attracting attention.

In this study, we tried to produce hydrogen from water/methanol photo-splitting using a core-shell structure catalyst. In particular, we proposed a CuS@CuInS₂:In₂S₃ catalyst with an interface between the core and the shell by controlling the structure and shape of the catalyst, this interface can act as a site where the catalyst can adsorb more reactants, thereby increasing the activity of the catalyst. The performance of CuS@CuInS₂:In₂S₃ catalyst containing sulfur vacancies due to structural defects was significantly higher than that of pure CuS and In₂S₃. As a result of H₂O-TPD, it was found that CuS@CuInS₂:In₂S₃ catalyst having interface can adsorb more reactants. In addition, PL and photocurrent measurements showed that the recombination between the photo-generated electrons and hole pairs of the CuS@CuInS₂:In₂S₃ catalyst was inhibited.

Revolutionizing Enhanced Oil Recovery: Prospects of Magnetized Water in Surfactant and Polymer Flooding

Marwan Y. Rezk^{*}, Soha E. Anwar and Nageh K. Allam

Energy Materials Laboratory (EML), American University in Cairo (AUC), Egypt

Abstract

Polymers and surfactants are the most widely used chemical flooding methods to enhance oil recovery. However, the high cost of chemicals is a growing barrier as the oil prices are decreasing. Nowadays, water can be magnetized at low cost to alter some of its properties including surface tension, pH, viscosity, and scale formation. The use of magnetized water under such altered properties would enhance the oil recovery through chemical enhanced oil recovery. In the work done, water has been magnetized by passing it through a high magnetic field (MF). Magnetized water has been characterized to compare it to distilled/deionized water as a reference by UV-Vis and Raman spectroscopy. Subsequent to magnetization, guar gum polymer has been dissolved in magnetized water and compared to another batch that is dissolved in the reference water. The thermal

stability of guar gum polymer was evaluated by thermogravimetric (TGA) analysis. On the other hand, magnetized water has been used versus oil to evaluate the interfacial tension reduction in comparison with the normal case in the presence of surfactant. The results have shown that the use of magnetized water can enhance the polymer's stability and reduce interfacial tension. The results promotes magnetized water to be a good candidate for cheaper enhanced oil recovery.

Effects of Milling Parameters on the Mechanical Properties of Multiwalled Carbon Nanotubes (MWCNTs) Reinforced Ti64 Nanocomposite Fabricated via Spark Plasma Sintering (SPS)

Oluwaniyi Ajiteru^{1*}, Thato Thshephe¹, Moses Okoro² and Peter Olubambi²

¹University of Johannesburg, South Africa

²Centre for Nanoengineering and Tribocorrosion, South Africa

Abstract

The discrete attributes of MWCNTs as related to their thermal, mechanical, and electrical behaviors has made them a suitable reinforcement for use in producing metal matrix composites (MMCs). The metal matrices can be Copper (Cu), Titanium (Ti), Magnesium (Mg), Aluminium (Al) and/or their alloys. Extensive research have shown that the produced composites possesses outstanding properties such as high corrosion resistance, high modulus of elasticity, high specific weight and strength which has made them to be employed in different applications for example in aerospace, marine, biomedical, petrochemical, and power amongst others. However, in the course of dispersing MWCNTs in metal matrices, it has been reported that several problems are being encountered some of which includes agglomeration of MWCNTs, breakage in the sp² structure of MWCNTs and formation of unwanted intermetallic compounds. Consequently, this adversely affects the properties of the nanocomposites. In this work, the synthesis technique used in dispersing MWCNTs of varying concentration (0.5 wt%, 1.0 wt% and 1.5 wt%) in Ti64 is high energy ball mill (HEBM). A batch (i, ii and iii) was formed for the dispersion using different milling parameters e.g. impact energy, ball-to-powder ratio (BPR), ball sizes, milling speed and time. The admixed powders were then fabricated via SPS with a pre-compaction force of 10 kN and at constant heating rate of 100 °C/min. The applied pressure and holding time utilized during the operation was 50 MPa and 5 min respectively in vacuum. The sintering temperature was varied between the range of 850 and 1000 °C. After investigation, it was observed that the mechanical properties of the produced nanocomposite depend greatly on the milling parameters.

The Influence of Oxygen Plasma Treatment on the Supercapacitors Characteristics of Sprayed-carbon Nanotube Thin Films

Shuo-Yang Weng^{*}, Yi-Chieh Li and Huang-Chung Cheng

Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan

Abstract

In this study, our goal is to fabricate a high-performance electrode based on CNTs for supercapacitors. We are using the ultrasonic spraying methods to fabricate the carbon nanotube-based supercapacitors. In order to increase the performance, the oxygen-containing functional groups acted as the redox reactions sites for extra capacitance. Hence, the increased amounts of these functional groups by increasing plasma treated time resulted in the improvement of the C_{sp}. In the end, an optimal condition was found at treatment time for 60s because the degree of oxygen-containing functional groups could be increased dramatically from 26.88% to 41.32% without over-damage on CNTs, resulting in the C_{sp} raising from 23.7 F/g to 49.3 F/g. The improvement ratio of C_{sp} was 2.1x in 1M Na₂SO₄ solution at a scan rate of 100 mV/s.

The Benzodithiophene-based Small Molecule for Ternary Organic Solar Cells with Non-fullerene Acceptors

Yi-Ju Lu^{*}, Yu-Che Lin, Hsiu-Cheng Chen and Kung-Hwa Wei

Department of Materials Science and Engineering, National Chiao Tung University, Taiwan

Abstract

Non-fullerene materials are new promising candidates for future application of organic solar cells. However, their low short-circuit current density (J_{sc}) limit the performance of power conversion efficiency (PCE). In this study, we replaced PC₇₁BM with non-fullerene materials (m-ITIC-OR) and introduced a simple concept of ternary blend system for organic solar cells. Small molecules (SM-⁴OMe) with complementary absorption spectrum were blended into the binary system (PTB7-TH:m-ITIC-OR) to successfully broaden the range of absorption spectrum and improve the J_{sc} of the non-fullerene ternary organic

solar cell device. The molecule structure of SM-4OMe is composed of a benzodithiophene (BDT) unit as the donor, which also in PTB7-TH leading to good morphology compatibility by blending PTB7-TH, SM-4OMe and m-ITIC-OR together to form desired packing orientation in the ternary blend films. Furthermore, fluorescence resonance energy transfer (FRET) effect is found between PTB7-TH and SM-4OMe, generating more carriers to diffuse to the interface so that the higher short-circuit current is collected and eventually the device was optimized. The best PCE of a device incorporating a ternary blend of PTB7-TH:SM-4OMe:m-ITIC-OR (0.9:0.1:1.5, w/w/w) as the active layer in chlorobenzene, was 8.61%. It is approximate 20% higher than the value 7.26% of the corresponding device incorporating binary blend of PTB7-TH:m-ITIC-OR (1:1.5, w/w). The ternary blend films with only a few amount of SM-4OMe ensuring the desired packing orientation for a better transportation of carriers. The result shows that the PCE for the single junction organic photovoltaics could be successfully enhanced by a facile procedure of ternary solar cells.

Tunable High Responsivity of Graphene-Si Field Effect Photodetector

Siwapon Srisonphan

Department of Electrical Engineering and ELectrons and Semiconductor Applications (ELSA) Laboratory, Faculty of Engineering, Kasetsart University, Bangkok, Thailand

Abstract

Carrier transport in two dimensional systems such as graphene and well-defined nanostructures can provide exceptional electronic characteristics. Due to the unique and remarkable physical properties, such as a high transparency to light and excellent carrier mobility, graphene has received considerable attention for future nanoelectronic and photonic applications. However, graphene-based photodetectors demonstrate low responsivity ($\sim 6\text{--}10$ mA/W) in the visible wavelength due to their weak optical absorption ($\sim 2.3\%$) and extremely short carrier lifetime. Herein, we present a photodetector based on graphene/SiO₂/Si (GrOS) field effect structure with an embedded nanoscale trench, allowing two devices (graphene/Si heterojunction and nanoscale vacuum based GrOS capacitor) combined at the same platform. The responsivity of the hybrid platforms based on p-Si and n-Si is fully and finely tunable up to 1.2 and 0.45 A/W, respectively, which correspond to external (internal) quantum efficiencies of 235% (350%) and 88% (132%), respectively. The multiple exciton generations (MEG) in the proposed device originate from the impact ionization initiated by photo-excited carrier injection into the self-induced localized electric field in Si. The primary mechanism of photoelectron transport is governed by ballistic electrons transport, which is emitted from the Si edge to graphene via a nanoscale air gap. We present both electrostatic current-voltage (I - V) characteristic and the transient response of hybrid photodetector. The integrated photodetector is architecturally Si-compatible and thus highly promising for ultrafast, low-power, and tunable responsivity for photonic applications.

Flexible Pressure Sensor with Double-layered Structure

Jinyoung Lee*, Dongkyun Shin, Gieun Kim and Jongwoon Park

Korea University of Technology and Education, South Korea

Abstract

The pressure sensor is used in various fields such as touch interface, health monitoring, artificial skin, etc. It should maintain the original function even in the bending or stretching state. In the case of devices that sense pressure through physical deformation by pressure, they can be easily damaged by soft contact. Therefore, it is necessary to maintain constant response characteristics to the change of the surrounding environment or repeated contact. Many studies have been made on capacitive pressure sensors since they have high sensitivity and stability. However, the production process of capacitive sensors is complicated and the cost is high. In contrast, the resistive pressure sensors are simple to fabricate and more cost effective. Even so, resistive pressure sensors show very poor sensitivity in the low pressure.

In this study, we have fabricated flexible resistive pressure sensors with nanometer-thick layers by spray coating using AgNWs and analyzed the electrical response. AgNWs are spray coated directly onto uncured polydimethylsiloxane (PDMS) such that AgNWs penetrate into the uncured PDMS, enhancing the adhesion properties of AgNWs. However, the AgNW sensor shows unstable electric response and low pressure sensitivity. Because of those issues, the conductive polymer, poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS), was coated on AgNWs to enhance the sensitivity and obtain stable electrical response. Such a double-layered sensor ensures a stable electric response because the PEDOT:PSS layer tellingly suppresses the protrusion of AgNWs from PDMS when pressure is applied.

Tunable Work Function of Metal Gate Stack by *In-situ* Atomic Layer Lamellar Doping of AlN in TiN

Kuei-Wen Huang*, Po-Hsien Cheng, Yu-Shu Lin, Chin-I Wang and Miin-Jang Chen

Department of Materials Science and Engineering, National Taiwan University, Taipei, Taiwan

Abstract

The work function of the Pt/Ti_{1-x}Al_xN_y bilayer metal gate electrode on the gate oxide was tailored by introducing a thin AlN-doped TiN interlayer using the *in-situ* atomic layer lamellar doping technique. With the increase of the nominal AlN lamellar doping percentage (DP_{AlN}) from 0% to 6.25%, the work function of the bilayer metal gate decreases from 4.49 eV and reaches a minimum of 4.19 eV. Then the work function increases to 4.59 eV as the DP_{AlN} increases to 50%. The Auger electron spectroscopy (AES) analysis reveals the linear dependence between the Al/(Ti+Al) concentration ratio and DP_{AlN} , indicating the capability of precise and digital control of the doping concentration and work function by the *in-situ* atomic layer lamellar doping technique. A low work function of 4.19 eV was achieved in the Pt/Ti_{1-x}Al_xN_y bilayer metal gate, which is appropriate as the low-work-function metal gate for n-MOSFET devices.

Patterning of Metallic Nanolines Based on Electron Beam Induced Deposition Accompanied with Selective Growth of Atomic Layer Deposition

Kuei-Wen Huang*, Po-Shuan Yang and Miin-Jang Chen

Department of Materials Science and Engineering, National Taiwan University, Taipei, Taiwan

Abstract

Patterning of nanoscale metallic structures is realized by the combination of electron beam induced deposition (EBID) and atomic layer deposition (ALD) techniques. Selective growth of the desired metallic material (Pt) on the seeding layer prepared by EBID is achieved by optimizing the ALD conditions. The electron dose required for the deposition of seeding layer is much lower, and the material quality of Pt nanolines is much improved by the selective ALD growth, as compared with those of the direct EBID. The method based on the EBID patterning and ALD selective growth provides an alternative way to improve the spatial resolution and material quality of the electron beam lithography.

Study on Organic Thin Film Coating for AMOLED Panel using Diluted Solution

Dongkyun Shin*, Jinyoung Lee, Gieun Kim and Jongwoon Park

Korea University of Technology and Education, Korea

Abstract

On the surface of the AMOLED, an insulator material such as a photo-resistor forms a bank for pixel defining. A capillary phenomenon occurs between ink and bank due to surface tension and adhesion force. It brings a concave thickness profile in which the pixel's center thickness is thin and the rim is thick. And degradation of emission uniformity within pixels.

With an attempt to suppress concave profile, we have performed slot-die coating with different concentration of aqueous PEDOT:PSS solution. In this work, we found that the dilution of solution affect to thickness uniformity by decreased film thickness of near bank edge. PEDOT:PSS was diluted with different ratio of DI water (de-ionized water) at 10:0, 7:3, 5:5, 3:7, respectively (PEDOT : water). As a result, thickness uniformity was measured as 51% using un-diluted PEDOT:PSS. As the concentration of PEDOT decreased, the in-pixel thickness uniformity gradually increased. The thickness uniformity of the 7:3 dilution and the 5:5 dilution was 67% and 69%, respectively. In the case of 3:7 diluted solution, the thickness uniformity was measured as 84%, which is the best result. When the solution is diluted, the drying time becomes relatively longer and the amount of the movable solution becomes larger. This micro fluid improves the thickness uniformity while reducing the thickness of the edge. In addition, the thickness uniformity can be controlled by the drying method. It was confirmed that the light emission of the AMOLED device is affected by the uniformity of the thickness with diluted solution.

Investigating the Optical Properties of Boron Nitride Nanotubes

Justin Anderson* and Lyons

Hampton University, Hampton, VA, USA

Abstract

This research paper presents developments in the investigation of the optical properties of boron nitride nanotubes such as

emission wavelengths and absorption peak. The experiment is designed to perform ultraviolet and Raman spectroscopy on an approximate isolated nanoliter of boron nitride nanotubes in an optical fiber sample tube. Over the course of the experiment, a simple, low-cost technique to isolate nanoliter samples of Boron Nitride nanotubes was created. Boron nitride nanotubes have already been investigated for their profound properties of high thermal conductivity, excellent mechanical strength, the emission of UV light and a tunable band gap that is stable regardless of small variations in diameter. The predetermined properties of boron nitride nanotubes and this experiment extend its field of applications.

Graphene Quantum Sheets with Multiband Emission: Unravelling the Molecular Origin of Graphene Quantum Dots

Radwa A. Shedeed^{*}, Ahmed S. Hassanien and Nageh K. Allam

Energy Materials Laboratory (EML), School of Sciences and Engineering, The American University in Cairo, New Cairo, Egypt

Abstract

The dependence of the fluorescence in graphene quantum dots on the excitation wavelength has been the focus of several studies recently. While some studies attributed their multi-chromophoric behavior to core and surface states, others related it to the differently-sized nanodomains of sp²-hybridized carbon in an amorphous matrix. Herein, colloidal graphene quantum sheets and nanoflakes were directly synthesized via low temperature catalytic chemical vapor deposition (CVD). These graphene nanostructures were found to exhibit well-resolved multi-emission bands in the visible region. Based on the X-ray photoelectron, FT-IR and Raman spectroscopies as well as density functional theory (DFT) calculations, the role of polycyclic aromatic hydrocarbons (PAHs) was identified as the building blocks of graphene quantum dots.

Flexible and Sensitive Humidity Sensor System based on Hydrophilic PTFE Thin Film for Real Time Detection

Uihyun Jung^{*}, Heekyeong Park, Seok Hwan Jeong, Muhammad Naqi, Na Liu and Sunkook Kim

School of Advanced Materials Science & Engineering, Sungkyunkwan University, Suwon, South Korea

Abstract

Recently, flexible electronics have attracted much more interests in versatile areas of fundamental sciences and industries. Flexibility is essential in many applications, where the sensor must be curved or subjected to repeated bends. Considering the flexible humidity sensor, it has multivariate impact on humans as well as on environment. Focusing on plant science, the relative humidity (RH) is most important for continuous monitoring of plant disorders during various process like photosynthesis, water absorbing. For this application, the sensor should have higher sensitivity, flexibility, and stability.

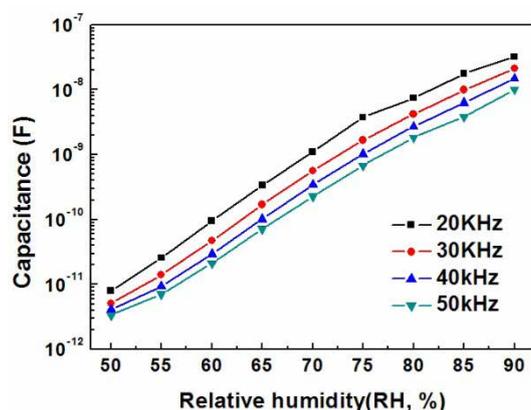


Figure 1: Capacitance variation of PTFE sensor with respect to RH.

In this work, we report on humidity sensing capability of flexible polytetrafluoroethylene (PTFE) sensor and the application to smart monitoring system. First, we presented a capacitive humidity sensor fabricated by using nanoporous PTFE substrate as sensing and frame material. The flexible humidity sensor exhibits a linear behavior in the range of 50 to 90 RH (%), shown in Figure 1. Flexible nature of PTFE film gives our sensor robust tolerance against mechanical stress, which was reinforced by adapting co-planar interdigitated electrodes. As a result, it shows no apparent degradation of device performance after up to 3,000 times of cyclic upward bending. Second, we demonstrated a real-time wireless monitoring system based on flexible PTFE

humidity sensor as data acquisition component. Bluetooth module connected by sensor enable wireless communication to smartphone. We demonstrated the functionality of our sensing system by attaching the flexible humidity sensor to a cylindrical surface and collecting data in real time.

Water-Soluble Iron Oxide Magnetic Nanoparticles (NPs) Coated by Biomaterials as Potential Negative Contrast Agents in Magnetic Resonance Imaging (MRI)

Alexandre D'Agostini Zottis¹, Eduardo Sant'Ana Ricardo¹, Brena Beatriz Pereira Ribeiro¹, Jeovandro Maria Beltrame², Mayara da Silva¹, Luiz Felipe Nobre³, Lucas Freiberger de Souza³ and Rozangela Curi Pedrosa²

¹Federal Institute of Education, Science and Technology of Santa Catarina – IFSC, Campus Florianópolis, Brazil

²Federal University of Santa Catarina – UFSC, Florianópolis, Brazil

³DMI Clinic –São José, Brazil

Abstract

Superparamagnetic of iron oxide nanoparticles (SPIONs) may be an alternative for replacing gadolinium-based contrast agents (GBCAs), since they could to cause nephrogenic fibrosis in patients with kidney problems according to FDA. Our research group is focused on studies for synthesize SPIONS coated by biomaterials and investigate features as negative CAs for helping to the detection of the early breast cancer. Then, we compared the SPIONs coated by polyethylene glycol (PEG) – (A01 and A02) with a type of melanin, named pheomelanin (C01). The infrared of A01 and A02 identified chemical group of Fe₃O₄, respectively (595.2 cm⁻¹ and 575.3 cm⁻¹) and peaks characteristic of PEG (-C-O-C at 1135 cm⁻¹ (A01) and 1124 cm⁻¹ (A02), CH₂ at 1400.5 cm⁻¹ (A01 e A02), also O-H at 3399.9 cm⁻¹ (A01) and at 3434.8 cm⁻¹ (A02)). Besides, for C01, the infrared indicated a band at 612 cm⁻¹ attributed to γ-Fe₂O₃, and other peaks corresponding to pheomelanin (O-H at 3138.8 cm⁻¹, C=O at 1621.7 cm⁻¹, C-O at 1001 cm⁻¹ and C-S at 617, 75 cm⁻¹). The DLS analysis indicated hydrodynamic sizes for all samples (less than 180 nm) and the EDS exhibited percentage indexes of iron and coating materials, confirming the formation of NPs. VSM analysis pointed out that the SPIONS A01 (22.2), A02 (65.0) and C01 (37.8) emu/g samples indicated superparamagnetic profile. Finally, for the measurements of MRI in T₂ weight, the effect of signal reduction for iron concentrations, respectively for R₂ (1/T₂), the slope value of samples C01, A01 and A02 was 217.8 ± 20.9, 198.2 ± 18.1 and 304.0 ± 22.1 (M⁻¹.s⁻¹), respectively. In conclusion, all samples as coating materials for SPIONs used as negative CAS were confirmed.

Freezing Decrease the Integrity of DNA Molecules

Ian C. Hsu

Department of Biomedical Engineering and Environmental Sciences, National Tsing Hua University, Taiwan

Abstract

DNA samples are commonly frozen for storage. However, freezing can compromise the integrity of DNA molecules. Considering the wide applications of DNA molecules in nanotechnology, changes to DNA integrity at the molecular level may cause undesirable outcomes. However, the effects of freezing on DNA integrity have not been fully explored. To investigate the impact of freezing on DNA integrity, samples of frozen and non-frozen bacteriophage lambda DNA were studied using optical tweezers. Tension (5 to 35 pN) was applied to DNA molecules to mimic mechanical interactions between DNA and other biomolecules. The integrity of the DNA molecules was evaluated by measuring the time taken for single DNA molecules to break under tension. Mean lifetimes were determined by maximum likelihood estimates and variances were obtained through bootstrapping simulations. The lifetimes of frozen DNA molecules are significantly reduced, implying that freezing compromises DNA integrity.

RNA Nanotechnology for Specific Delivery of Anti-miRNA for Suppression of Breast, Prostate and Brain Cancer

Dan Shu¹, Daniel Binzel¹, Tae Jin Lee², Hongran Yin¹, Yi Shu^{3,4}, Hui Li¹, Ren Xu^{4,5}, Bin Guo⁶, Carlo M. Croce² and Peixuan Guo^{1,7,8}

¹Pharmaceutics and Pharmaceutical Chemistry, College of Pharmacy, The Ohio State University, Columbus, OH, USA

²Department of Cancer Biology and Genetics, College of Medicine, The Ohio State University, Columbus, OH, USA

³College of Pharmacy, University of Kentucky, Lexington, KY, USA

⁴Markey Cancer Center, University of Kentucky, Lexington, KY, USA

⁵Department of Molecular and Biomedical Pharmacology, University of Kentucky, Lexington, KY, USA

⁶Department of Pharmaceutical Sciences, North Dakota State University, Fargo, ND, USA

⁷Department of Physiology & Cell Biology, College of Medicine, The Ohio State University, Columbus, OH, USA

⁸Dorothy M. Davis Heart and Lung Research Institute, The Ohio State University, Columbus, OH, USA

Abstract

MicroRNAs (miRNAs) are non-coding RNA molecules that regulating post-transcriptional gene expression and cellular differentiation, proliferation and apoptosis. The oncogenic microRNA-21 gene (miR-21) has been identified commonly overexpressed in solid tumors such as breast, lung, prostate, colon, brain cancers etc. Knocked down miR-21 expression by anti-miR21 has been proposed to treat solid tumors by up-regulating tumor suppressors, PTEN and PDCD4. However, delivery of anti-miR21 to the tumor without collateral damage requires an efficient and robust platform. Here, we report the application of RNA nanotechnology using three-way-junction (3WJ) nanoparticles derived from phi29 DNA packaging motor for specific delivery of anti-miR21 and to inhibit the growth of breast cancer, prostate cancer and brain cancer. Utilizing the thermodynamic ultra-stable 3WJ motif, multivalent RNA nanoparticles were constructed incorporating target ligands (such as Folate or PSMA and EGFR RNA aptamers) and high thermodynamic stable anti-miR21 seed as therapeutic module. The RNase resistant and thermos-dynamically stable RNA nanoparticles remained intact after systemic injection in mice and strongly bind to tumors with little accumulation in health organs eight hours' post-injection. The use of 20 nM RNA nanoparticles with 54nt 3WJ, 8nt anti-miRNA seed and 30-40 nt RNA targeting aptamers will enhance tumor regression effect. RNA nanotechnology exhibits clinical potentials as a platform for targeted cancer treatment.

Design and Evaluation of Self-assembled Scaffolds using Biodegradable Polymer Microparticles

Akansha Singh^{*}, Prasad Admane, Robin Kumar and A. K. Panda

National Institute of Immunology, New Delhi, India

Abstract

Scaffold fabrication method is momentous as it helps in defining the porous architecture and mechanical strength of the scaffold. The major problem associated with scaffold manufacturing techniques is loss and degradation of incorporated biostimulatory molecules, such as growth factors, drug or enzymes. A new method of scaffold fabrication using PDLA polymer was designed earlier in our lab. This method ensures limited loss of functional ability of the entrapped molecules. The labile biomolecules stay encased inside the fused particles and can be delivered through the scaffold in a controlled fashion. We have successfully entrapped antibiotics like Gentamycin and Neomycin inside scaffold particles. Antibiotic released from the scaffolds was found to be bioactive as tested against *Staphylococcus aureus* and the release pattern was biphasic over a period of one week. We have prepared scaffolds with different mechanical properties using nano-sized, micro-sized and macro-sized polymeric particles. The scaffolds were found to be non-toxic to murine fibroblasts cultures *in vitro* as well as to mice upon subcutaneous implantation. This method provides a novel and easy way of fabricating antibiotic loaded polymer scaffolds for varieties of applications. Furthermore, these scaffolds can be used for targeted delivery of drugs and growth factors encapsulated in polymeric nano- or micro-particles fused to form a membrane.

Ultrastructure of the Gut and Testis in *Acheta domesticus* after Exposure to Graphene Oxide in Food

Marta Dzięwiecka¹, Barbara Flasz¹, Julia Karpeta-Kaczmarek¹, Magdalena Rost-Roszkowska² and Maria Augustyniak¹

¹Department of Animal Physiology and Ecotoxicology, University of Silesia in Katowice, Katowice, Poland

²Department of Animal Histology and Embryology, University of Silesia, Katowice, Poland

Abstract

Market analysis unambiguously shows that materials of graphene family will be more and more often employed in industry, medicine and food production. Defining potential threats of new substances for organisms on an early stage of their production and implementation is a primary task of modern medicine, toxicology and ecotoxicology.

The main research problem of our project is assessment of influence of graphene oxide (GO) on the selected vital parameters of a model insect species *Acheta domesticus*.

In this research we attempted to investigate short-term *in vivo* toxicity of graphene oxide. The nanoparticles were administrated to *Acheta domesticus* with food during ten days of adult individuals.

The total oxidative stress was checked at the beginning and at the end of the experiment using flow cytometry. A histological assessment of the gut and male gonad (testis) was performed after ten days of treatment using Transmission Electron Microscopy (TEM). The results reported intensification of oxidative defense and numerous degenerative changes in the tissues of *Acheta*

domesticus (especially in the midgut and testis). We can therefore assume that graphene oxide can migrate via the epithelium to hemolymph, and then can be distributed throughout the whole organism.

Acknowledgment: The research was supported by the National Science Centre (NCN) on the basis of Agreement No. UMO-2016/23/N/NZ7/01977.

Electrically Controlled Drug Release from Drug Loaded Polymer Nanocomposite Films

Christian Chamberlayne¹, Ephraim Neumann² and Richard Zare¹

¹Stanford University, CA, USA

²Leibniz University Hannover, Germany

Abstract

Medical implants capable of releasing quantitative amounts of drugs on demand open many possibilities in medical device applications. Toward this goal, we have developed drug loaded polymers that release drugs upon electrical stimulation. The polymer acts both as a drug reservoir and a release mechanism for medical implants. The ease at which electronics can be miniaturized as well as the quantitative control on amount of released drug through the voltage and current are two large advantages for electrically stimulated drug release.

Two issues facing the field of electrically stimulate drug release are: loading sufficient quantities of drug, and releasing said drug with low voltages. We demonstrate drug loadings above 40% by weight as well as drug release at low voltages (less than 1.5V). Our system is also quite versatile, allowing electrically stimulated drug release of a variety of drugs, spanning from small molecules up to small polypeptides like insulin.

Nanoprobes Displaying Surface Enhanced Raman Scattering Signals for the Multiplexed Detection of Protein Biomarkers

In-Jun Hwang^{*}, Jin-Kyoung Yang, Tae Woog Kang and Jong-Ho Kim

Department of Chemical Engineering, Hanyang University, Ansan, South Korea

Abstract

It is of importance to detect protein biomarkers in a sensitive and multiplexed manner for the early and accurate diagnosis of diseases. Herein, we present an approach for designing surface-enhanced Raman scattering (SERS) nanoprobes with various optical signals for the sensitive and multiplexed detection of the potential biomarkers of Alzheimer's disease (AD). For the synthesis of the SERS nanoprobes, silver nanoshells (AgNSs) were rapidly formed on the surface of silica nanoparticles via the Raman labels-assisted reduction of Ag ions under very mild conditions (25 °C and 60 min). As-prepared SERS nanoprobes had uniform AgNS with a 50 nm of thickness and a 2 nm of nanogaps for electric field enhancement. The SERS nanoprobes exhibited strong Raman signals with the enhancement factor of 1.7×10^7 . In addition, each SERS nanoprobe displayed its own Raman signal without overlapping. The SERS nanoprobes conjugated with antibodies were then applied for the sensitive and multiplexed detection of Alzheimer's disease (AD) biomarkers, such as A β 40, A β 42, and total tau proteins. It was found that the SERS nanoprobes were capable of detecting all the proteins at concentrations as low as 1 pg/ml in a multiplexed manner.

Graphene Oxide can Cause Multigenerational Harmful Effects

Marta Dzięwiecka¹, Barbara Flasz¹, Julia Karpeta-Kaczmarek¹, Jolanta Kwaśniewska² and Maria Augustyniak¹

¹Department of Animal Physiology and Ecotoxicology, University of Silesia in Katowice, Katowice, Poland

²Department of Plant Anatomy and Cytology, University of Silesia in Katowice, Katowice, Poland

Abstract

Graphene oxide (GO) – an oxidized derivative of graphene, has been acclaimed a “superstar” in the area of nanomaterials in recent years. It draws researchers' attention with a number of its unique physicochemical properties which determine its potentially widespread use in industry, science and medicine. Therefore, potential influence of graphene and its derivatives on environment is a burning issue nowadays. It seems obvious that nanoparticles can penetrate to the organism via many different ways. But still, knowledge about effects of long-term exposure of organism to nanoparticles, including GO, is rudimentary. In the long-term perspective the knowledge will influence progress of the civilization through determining potentially unfavorable consequences and contribution in assessing risk associated with use of graphene oxide, both for human and other organisms.

In our study we focused on long-term *in vivo* toxicity of graphene oxide. Two generations of house cricket (*Acheta domesticus*)

Abstract

Lately, the attention towards multiple modality imaging with nanostructured contrast agents have rapidly grown thanks to the remarkable properties displayed by metallic nanostructures. Herein we report the synthesis of a resilient nanosystem based on silica-coated magnetic MnFe_2O_3 nanoparticles conjugated to fluorescein and PEGylated gold nanorods embedded in polymeric micelles ($\text{MnFe}_2\text{O}_4@\text{SiO}_2@\text{GNRs@PMs}$), for magnetic-photoacoustic-optical triple-modality imaging. The magnetic relaxivity of the nanosystem has been evaluated, revealing high r_2/r_1 ratios that suggests the effectiveness of the nanosystem as T_2 -contrast agent with MRI instrumentations commonly implemented at clinical stage. In addition, contrast-based fluorescence imaging has been tested both *in vitro* and *ex vivo*, showing that the nanosystem owned the suitable optical properties of fluorescein, with contrast intensities comparable with previously reported results. Finally, photoacoustic performances of the nanosystem have been evaluated, revealing good linearity between concentration and photoacoustic response in the 25 – 250 nM concentration. Furthermore, the performances of $\text{MnFe}_2\text{O}_4@\text{SiO}_2@\text{GNRs@PMs}$ for PA imaging have been tested *ex vivo* and *in vivo* with irradiation at 690 nm. The results showed a contrast-to-noise ratio (CNR) as high as 60 in a mouse leg subcutaneously injected with the nanosystem. The inner Mn-Ferrite core allowed for efficient MRI, the conjugation to fluorescein guaranteed sensitive detection by optical imaging and the presence of gold nanorods ensured enhanced photoacoustic contrast in the first biological window of the NIR spectrum, both *in vitro* and *in vivo*. Biocompatibility studies revealed no hemolytic effect induced by the nanoconstruct, revealing the applicability of the studied diagnostic tool for medical studies at the clinical stage.

Two-dimensional Nanosheet Biosensors for the Optical Detection of Pathogens

Tae Woog Kang*, Juhee Han, Sin Lee, In-Jun Hwang, Su-Ji Jeon, and Jong-Ho Kim

Department of Chemical Engineering, Hanyang University, South Korea

Abstract

It is of great interest to modulate the dimension of nanomaterials for their biological applications. Herein, we present an effective approach for the exfoliation and functionalization of transition metal dichalcogenides (TMDs) such as WS_2 , MoSe_2 , and WSe_2 with a recognition chemical element in an aqueous solution, and the application of exfoliated TMD monolayers for the selective detection of bacterial pathogens. Bulk TMDs were effectively exfoliated into TMD monolayers using a polysaccharide polymer in water via a pulse sonication process. The obtained TMD monolayers exhibited characteristic excitonic absorption and strong fluorescence in a visible range, as compared with their bulk counterparts. The TMD monolayers displayed their characteristic Raman scattering signals and the vibrational modes of the polymer in the Raman and FT-IR spectra, indicating that the exfoliation and functionalization of the TMD monolayers in an aqueous solution were successfully achieved. The TMD monolayers were then applied for the selective detection of bacteria without the use of antibodies. The WS_2 monolayers were able to selectively detect *E. coli* at concentrations as low as a single copy.

Cytotoxic Evaluation of HDAC Inhibitor Conjugated Prodrug Micelles for Doxorubicin Delivery against Lung Cancer

Bolutito Alade¹, Ying Xie² and David Oupicky²

¹Hampton University, Hampton, VA, USA

²University of Nebraska Medical Center, Omaha, NE, USA

Abstract

Colon cancer is the third most prevalent cause of cancer-related death and the second most common form of cancer in the United States. In colon cancer, as well as many other cancer types, the tumor suppressing gene p53 is typically subject to inactivation or mutation. Suppression of p53 leads to the dysregulation of the different classes of microRNAs. Among them, the upregulation of mi-34a induces cell apoptosis and/or cell cycle arrest in both cancerous and defective cells. The goal of this study was to characterize a newly developed hydroxychloroquine-conjugated polycation (HQ-P) in comparison with the parent polycation (P), as well as study each one's ability to deliver miRNA in HCT116 human colon cancer cells. The hypothesis for this study was that both delivery systems will have relatively similar physiochemical properties (size, ζ potential, miRNA loading capacity), but the HQ-P-based systems will demonstrate higher endosomal escape activity and cell apoptosis in cultured HCT116 cells.

RNA Nanoparticles Delivering Therapeutics for Thyroid, Prostate, Breast and Brain Cancer Treatment

Congcong Xu*, Peixuan Guo, Sissy Jhiang and Dan Shu

The Ohio State University, OH, USA

Abstract

With the effective treatment of most thyroid cancer by total thyroidectomy and radioiodine ablation, 10% - 20% of the cases remain challenging due to the resistance to conventional chemotherapy and radioiodine therapy. New strategies with enhanced and prolonged therapeutic efficacy are urgently needed. Herein, we developed RNA nanotechnology-based system for therapeutic RNA delivery into thyroid cancer cells for effective cell inhibition. Specifically, a three-way junction (3WJ) motif derived from the packaging RNA (pRNA) of phi29 DNA packaging motor was engineered to harbor EGFR aptamer and anti-miRNA 21 for targeted delivery. Flow cytometry analysis showed the specific binding of RNA nanoparticles to the thyroid cancer cells and the q-RT PCR results suggested the successful gene regulation. We envision that this 3WJ-based therapy platform holds great promises for radioiodine- and chemotherapy-refractory thyroid cancer.

RNA-based Micelles: A Novel Platform for Paclitaxel Loading and Delivery

Yi Shu¹, Hongran Yin^{2*}, Mehdi Rajabi¹, Hui Li², Mario Vieweger², Sijin Guo², Dan Shu² and Peixuan Guo²

¹Nanobiotechnology Center, Markey Cancer Center and Department of Pharmaceutical Sciences, University of Kentucky, KY, USA

²Center for RNA Nanobiotechnology and Nanomedicine, College of Pharmacy, Division of Pharmaceutics and Pharmaceutical Chemistry, College of Medicine, Dorothy M. Davis Heart and Lung Research Institute and James Comprehensive Cancer Center, The Ohio State University, Columbus, OH, USA

Abstract

RNA can serve as powerful building blocks for bottom-up fabrication of nanostructures for biotechnological and biomedical applications. In addition to current self-assembly strategies utilizing base pairing, motif piling and tertiary interactions, we reported for the first time to build RNA based micellar nanoconstruct with a cholesterol molecule conjugated onto one helical end of a branched pRNA three-way junction (3WJ) motif. The resulting amphiphilic RNA micelles consist of a hydrophilic RNA head and a covalently linked hydrophobic lipid tail that can spontaneously assemble in aqueous solution via hydrophobic interaction. Taking advantage of the feature of pRNA 3WJ branched structure, the assembled RNA micelles are capable of escorting multiple functional modules. As a proof of concept for delivery for therapeutics, Paclitaxel was loaded into the RNA micelles with significantly improved water solubility. The successful construction of the drug loaded RNA micelles was confirmed and characterized by agarose gel electrophoresis, atomic force microscopy (AFM), dynamic light scattering (DLS), and fluorescence Nile Red encapsulation assay. The estimate critical micelle formation concentration ranges from 39 nM to 78 nM. The Paclitaxel loaded RNA micelles can internalize into cancer cells and inhibit their proliferation. Further studies showed that the Paclitaxel loaded RNA micelles induced cancer cell apoptosis in a Caspase-3 dependent manner but RNA micelles alone exhibited low cytotoxicity. Finally, the Paclitaxel loaded RNA micelles targeted to tumor *in vivo* without accumulation in healthy tissues and organs. There is also no or very low induction of pro-inflammatory response. Therefore, multivalence, cancer cell permeability, combined with controllable assembly, low or nontoxicity nature, and tumor targeting are all promising features that make our pRNA micelles a suitable platform for potential drug delivery.

Protease-Activatable Polymersomes for Diagnostics and Treatment of Cancer Cell

Hyun-Ouk Kim^{1*}, Hyeoung Son², Jong-Woo Lim¹, Jihye Kim¹, Haejin Chun¹, Geunseon Park¹, Yong-Min Huh¹ and Seungjoo Haam¹

¹Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, South Korea

²YUHS-KRIBB Medical Convergence Research Institute, Seoul, South Korea

Abstract

Metastasis-associated proteases, such as MT1-MMP, play decisive roles during malignancy and have been used as biomarkers for diagnosis, prognosis, and drug targeting. Proteases-activatable polymersomes have great potential as cancer theragnosis platform due to the high selectivity of the activating proteases. Here we report a highly modular design for the efficient and simple synthesis of amphiphilic block polymer-peptide and copolypeptide based on methoxy-poly (ethyleneglycol)-b-poly-leucine (mPEG-b-pLeu) and MT1-MMP antagonist peptide-b-poly-leucine (MT1-peptide-b-pLeu), respectively. These amphiphilic self-assemble in water into polymersomes that can disassemble and release encapsulated imaging agent, gene and drug upon enzymatic activation. Importantly, this system was found to prevent the initiation and progression of cancer

metastasis. Consequently, this study may also provide new strategy in the development of nanomedicine for diagnosis and therapy of cancer metastasis.

Silver Nanoparticles as Antibacterial against Fish Bacterial Diseases

Julio César Meneses^{1*}, Aida Handam¹, María del Carmen Monroy² and Jorge Castro²

¹Laboratorio de Microbiología y Biología Molecular del Departamento de Atención a la Salud, Universidad Autónoma Metropolitana Unidad Xochimilco, Mexico

²Laboratorio de Alimento Vivo y Análisis Químico del Departamento del Hombre y su Ambiente, México City, Universidad Autónoma Metropolitana Unidad Xochimilco, Mexico

Abstract

Nanotechnology is a field of research of the nanoparticles due to their noble properties within that highlight its antimicrobial effect, in particular silver nanoparticles [1]. The use of silver as an antibacterial has been since ancient times. In aquaculture, the ornamental fish have expressed bacterial diseases, which have resistance to the different types of antibiotics [2]. The aquaculture industry are looking for new alternatives for the control of these diseases [3]. The aim of this work is to determine the antibacterial effect of silver nanoparticles (AgNPs) against *Vibrio fluvialis*. The AgNPs were synthesized at different concentrations (180 and 90 ppm) using sodium citrate as a reducing agent. The Turbidimetric assay [4] results shown that AgNPs could inhibit the grown of *V. fluvialis*, in concentration depended manner. The minimum inhibitory concentration (MIC) of AgNPs against *V. fluvialis* was 45 ppm. Toxicity results [5] prove that AgNPs are not toxic to Angel fish (*Pterophyllum scalare*). There was no harm in eyes, fins and scales. This study concluded that the AgNPs showed antibacterial activity against *V. fluvialis*. However, future studies of the effect of AgNPs are necessary in other pathogenic microorganisms, which affect the health of the ornamental fish.

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Identifying the Critical Amino Acids within Immunoglobulin Domain of Human Peroxidase Necessary for Crosslinking of Basement Membranes

M. Gaines-Smith*, T. Maitre and I. Ero-Tollive

Hampton University, Hampton, VA, USA

Abstract

Assembly and integrity of collagen IV networks is essential for the integrity of basement membranes. An integral component of collagen IV is the sulfilimine bond (S = N), between methionine-93 and hydroxylysine-211 within the NC1 domains. This bond was identified as important for stabilization of basement membrane networks. Peroxidase has been identified as the multi-domain peroxidase responsible for catalyzing sulfilimine bond formation by using its peroxidase and n-terminus of the immunoglobulin (Ig) domain. Previously, we identified the peroxidase and immunoglobulin domain as the domains necessary for crosslinking the basement membrane. Therefore, our current work focuses on investigating and identifying the critical amino acids within the immunoglobulin domain of peroxidase responsible for catalyzing sulfilimine bond formation. To this end, we are designing primers to introduce specific mutations into our target Ig site within peroxidase. These mutants will later be transfected into HEK293T cells that are overlaid on uncrosslinked basement membrane generated by PFHR-9 cells. Using SDS-PAGE, western blots and commassie staining we will assess the amount of crosslinking to determine the critical amino acids of the immunoglobulin domain of peroxidase that is necessary and sufficient for crosslinking the basement membrane. These findings will provide insight into the mechanism for crosslinking/sulfilimine bond formation within the basement membrane.

Self-assemble Dynamics and Nanostructural evolution of a Novel Amphiphilic Chitosan for Drug Encapsulation and Release upon Anti-cancer Treatment

Min-Chin Chang*, Wei-Ting Huang, Ming-Chia Li and Dean-Mo Liu

Department of Materials Science and Engineering, Nano-Bioengineering Lab, National Chiao Tung University, Taiwan

Abstract

Self-assembly has been an interesting and important dynamic behavior for a materials possessing amphiphilic nature, and this is frequently observed in nature. What is more critical and also a need to explore while its association with drug molecule(s), for encapsulation and release in order to achieve a better-than-ever medical efficacy, compared with conventional free-drug medication protocol. Here, we employ a novel amphiphilic biodegradable and biocompatible materials, carboxymethyl-hexanoyl chitosan (termed as CHC), which has been successfully synthesized from this lab. The self-assemble dynamics and nanostructural evolution of the CHC in the presence and absence of hydrophobic drug were intensively explored through the use of H-NMR, C-NMR, FTIR, DLS, TEM, circular dichroism (CD) and small-angle electron diffraction. The stability of the self-assembled nanostructure was measured and was found to become dynamic with drug presence, suggesting drug release lead to a nanostructural variation over a certain extent. A corresponding drug release dynamic was then characterized in this work and a full explanation on nanostructure-associated drug elution from a given nanocarrier was proposed, which will be important with respect to nanomedicinal design from molecular consideration. This work also confirmed a nanostructural stability and minimized critical micellar concentration, and high encapsulation efficiency for anti-cancer drug, ensuring a potential benefit for the CHC in biomedical applications.

Non-aqueous Type Biosensor Based on Double Gate MoS₂ Field-effect Transistor for High Sensitive and Reproducible

Seok Hwan Jeong*, Heekyeong Park, Uihyun Jung and Sunkook Kim

School of Advanced Materials Science and Engineering, Sungkyunkwan University, South Korea

Abstract

Label-free, high sensitivity, and rapid detection are utmost valuable advantages of biosensors based on field-effect transistor (FET). Among various semiconductor channel materials, two dimensional materials, such as graphene and transition metal dicalcogenides (TMDs), have great potential for ultrahigh sensitive biosensor due to their large surface to volume ratio. Compared with graphene based FETs, TMDs based FETs are more effectively controlled by binding of biomolecules due to the existence of bandgap.

In this work, a molybdenum disulfide (MoS₂) FET based biosensor was used for high sensitive prostate specific antigen (PSA) detector. The detection of PSA was occurred on surface of MoS₂ passivated with Al₂O₃ top dielectric layer. This top layer was coated with high dense and well-oriented anti-PSA. Non-aqueous measurement process was selected for enhancement of both sensitivity and reproducibility. The pH memory theory, the proteins maintain their ionization state after removing aqueous, is a great theoretical tool of our detection systems. Non-specific binding between Al₂O₃ above MoS₂ surface and other molecules was perfectly suppressed with casein blocker for high reliability. The ultrahigh sensitivity of our MoS₂ biosensor was proved with much low limit of detection of 100 fg/mL. Finally, theoretical simulation suggested that optimization of device parameter such as thickness of Al₂O₃ layers offers the more enhanced performance of biosensor such as sensitivity and power-efficient.

Survival Fraction and RBE for X-ray Irradiated MDA-MB-231 Cell Culture with Intracellular Gold Nanoparticles: An Analytical Framework for the Assessment of the Cell Survival

Wilmer Melo-Bernal*, Marcelino Barboza-Flores and Valery Chernov

Universidad de Sonora, Mexico

Abstract

The uses of gold nanoparticles (GNPs) as radiosensitizers have been widely explored during the last years. *In vitro* and *in silico* experiments have demonstrated a significant dose enhancement in the GNP vicinity and reduction in cell survival under X-ray irradiation. The dose enhancement due to GNPs is attributed to a large photoelectric cross section of gold at the K-shell, which leads to the increase in the number of lethal lesions in critical cell structures. Although the physical mechanisms of the energy deposition are understood, at present the reasons for the biological outcomes are not clear.

The GNP distribution in a cell is the most important factor that determines the dose delivered to the cell nucleus and the

probability of the cell survival. In this work, we use an analytical framework for the assessment of the cell survival proposed in [1], which is based on the Local Effect Model, allowing us to take into account the effects of highly inhomogeneous dose distribution in the nucleus due to the intracellular distribution of 20 nm GNPs. The survival fraction curves and the RBE of MDA-MB-231 cell structure irradiated with 100 keV X-rays were calculated using the published radial dose distributions around the GNPs and specific distributions of GNPs in cells. As a result, a set of survival curves and corresponding RBE were obtained that reasonably coincides with the data available in literature.

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In-planta Quantum Dots Translocation via Rolling

Yasmine AbdEllatif¹, Andrew Towers², Tyler Maxwell^{1,2}, Swadeshmukul Santra¹⁻⁴ and Andre Gesquiere^{1-3,5}

¹NanoScience Technology Center, University of Central Florida, Orlando, FL, USA

²Department of Chemistry, University of Central Florida, Orlando, FL, USA

³Department of Materials Science and Engineering, University of Central Florida, Orlando, FL, USA

⁴Burnett School of Biomedical Sciences, University of Central Florida, Orlando, FL, USA

⁵The College of Optics and Photonics (CREOL), University of Central Florida, Orlando, FL, USA

Abstract

This work is focused to identify and confirm the translocation of the quantum dots within the citrus plant vascular tissue. This will be achieved by inducing pores in the stem region via roller, to permit the entrance of the quantum dots to the inside tissue. Plant branches were brought and treated as follows: rolled /covered with quantum dots, rolled /covered with water and non-rolled/ covered with quantum dots. Plants were dissected at the stem region and one section was obtained from each plant. Sections were examined by fluorescence lifetime imaging (FLIM), time correlated single photon counting (TCSPC) and optical microscopy imaging. It was found that the rolled sample with quantum dots acquired the quantum dots through the induced pores and translocated through the tissue. This is clearly appeared from the fluorescence lifetime values, TCSPC decay curves and the optical images (Figure 1). In conclusion, the induction of pores via roller with adding sufficient amount of quantum dots solution and prevent its dryness, ensures the quantum dots uptake and translocation into the plant instead of the gauze/ Swiffer® quantum dots treated plants only.



Figure 1: The optical microscope images (10X) for (A) rolled /covered with water sample (Control) and (B) rolled /covered with quantum dots sample. The blue arrow shows the quantum dots.

Synergistic Therapeutic Efficacy Using Dual-drug Co-delivery to Against Non-Small-Cell Lung Cancer: From *In-vitro* to *In-vivo*

Yi-Hsin Chen¹, Yu-Chian Chiang, Wei-Ting Huang and Dean-Mo Liu

Department of Materials Science and Engineering, Nano-Bioengineering Lab, National Chiao Tung University, Taiwan

Abstract

A novel dual-drug co-delivery nanosystem was successfully developed using carboxymethyl-hexanoyl chitosan (CHC) as a nanocarrier, through self-assembly co-encapsulation process designed in this work, for the treatment of advanced non-small-cell lung carcinoma (NSCLC, A549). A combination therapy with co-dosing of two drugs simultaneously with different mechanisms of action toward the disease site renders a synergistic therapeutic performance feasible. This has been confirmed

in our work where a combination of chemo-drug, gemcitabine (dFdC), which effectively inhibit DNA formation, leading cell death, and a Chinese herbal drug, demethoxycurcumin (DMC), which is able to downgrade NF-kB expression and reduce largely the multi-drug resistance (MDR) mechanism, gave rise to a synergistic cell-killing performance, in terms of a measure of combination index. The same protocol was designed for in-vivo evaluation with a further modification with targeting moiety, EGFR antibody, on the co-delivery nanocarriers and a significantly enhanced inhibition on tumor growth was observed in a mice model, which further justified the co-delivery efficacy proposed in this work. Co-encapsulation and associated self-assembly behavior of the CHC nanocarrier were systemically explored and an optimized synthesis protocol for this dual-drug co-loaded system was experimentally determined in full. It is believed, from this work, optimization of the co-delivery nanosystem largely enhance therapeutic efficacy compared to either free drug or sequentially-delivered (one drug after another) dosing protocols. Our finding can then envision a future development on the use of anticancer drugs, either chemotherapeutic or possibly immunotherapeutic drugs, with optimal combination strategy in treating advanced tumor progression with greater performance and is highly feasible in clinical translation.

Design and Synthesis of Amphiphilic Acrylic-chitosan Macromolecule and its Association with Hydrogel Lens for Anti-glaucoma

Yunru Hsieh and Dean-Mo Liu

Department of Materials Science and Engineering, Nano-Bioengineering Lab, National Chiao Tung University, Taiwan

Abstract

This work aimed at designing amphiphilic acrylic-chitosan macromolecule with self-assembly and water affinity properties to associate with hydrogel-based contact lens to treat glaucoma with enhanced efficacy and bioavailability. A newly-formed carboxymethyl-hexanoyl chitosan (termed as CHC) has been successfully developed from this lab for years. Its amphiphilic nature permitted a self-assembly nanostructure to evolve in aqueous media, and in the meantime, allows bioactive drug(s) to be encapsulated and delivered in a controlled, sustained manner for medication purpose. Combining the CHC, also a mucoadhesive biomaterials, with contact lens brings a new therapeutic strategy to treat eye disease, in particular, glaucoma. However, the lack of interfacial bonding between CHC and contact lens, either Poly-HEMA hydrogel or silicone-based hydrogel, reduced its mechanical integrity, water affinity (retention capability), and even optical clarity. Therefore, an attempt was made to link acrylic molecule with CHC via a chemical bonding, and from our work, it is being successfully synthesized a HEMA-conjugated CHC nanostructure (termed as H-CHC), without changing self-assembly nature and water affinity as of original CHC. Further association with poly-HEMA results in a high-clarity hydrogel lens, with much improved mechanical behavior, and high water retentionability. Encapsulating anti-glaucoma drug (with both single- and dual- drug protocols), a sustained release of the drug(s) from the resulting contact lens ensures a long-term control of intraocular pressure to a healthy level, between 15-20 mmHg and it is highly expecting the resulting drug-eluting contact lens can be successful in clinical translation.

Improving the Hydrogen Production in Water Splitting by a Simple Hot-press Process and Spontaneous Spatial Charge Separation Effect

Wei-Hsuan Hung*, Chien-Jung Peng, Kun-Lin Yang, Sz-Nian Lai and Chin-Ru Yang

Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan

Abstract

In this study, a spontaneous charge spatial separation (SCSS) and simple hot press process (HPP) has been adopted to enhance the efficiency of photocatalytic water splitting. Originally, the photocatalytic activity of hematite is limited by its relatively poor absorptivity, very short excited-state lifetime, and a short hole diffusion length. To address these issues, pseudocubic polyhedral α -Fe₂O₃ photoelectrode was fabricated and achieved the spontaneous charge spatial separation in water splitting process. The intrinsic charge spatial distribution has to be taken into account when selecting the facets, as it results in accumulation of photoexcited electrons and holes on certain semiconductor facets. Furthermore, we develop a new technology of using a simple hot press process to improve carrier transport, charge separation and longtime stability for photocatalytic water splitting. Without complicated nanostructure fabrication, this hot press process demonstrated a 2-fold enhanced photocurrent under A.M. 1.5 solar simulator irradiation. The enhancement is attributed to the improvement of carrier transport properties in TiO₂-Fe₂O₃ matrix due to significant reduction of the film thickness after the hot press process. In addition, Tin (Sn) from the FTO substrate was diffused and doped into these polyhedral α -Fe₂O₃ and hot press TiO₂-Fe₂O₃ during the sintering process to serves as an electron donor and increases the carrier density. In addition, plasmonic gold nanoparticles were incorporated into these two systems, which would provide the strong field and hot electrons, resulting in the enhancement of visible light absorption efficiency and inhibit charge recombination, this leads the photocatalytic water splitting to achieve a further stage.

Electro-spun C/Ge/GeO₂-based Fibrous Membranes as Binder-free Anode Materials for Flexible Li-Ion Batteries

Saveria Santangelo¹, Fabiola Pantò², Yafei Fan³, Sara Stelitano⁴, Patrizia Frontera¹, Pierluigi Antonucci¹, Salvatore Patanè⁵ and Nicola Pinna³

¹Mediterranean University, DICEAM, Reggio Calabria, Italy

²Mediterranean University, DIIES, Reggio Calabria, Italy

³Humboldt-Universität, Berlin, Germany

⁴Calabria University, DF, Arcavacata di Rende, Italy

⁵Messina University, MIFT, Messina, Italy

Abstract

The ever-increasing demand of wearable/bendable electronics has promoted the research in the field of flexible Li-ion batteries (f-LIBs). Germanium oxide (GeO₂) is a promising high-capacity anode material for LIBs (theoretical capacity: ~1126 mA h/g) [1]. However, it suffers from poor cyclability due to the huge volume changes during the lithiation/delithiation process. As known, encapsulating oxide nanoparticles within a three-dimensional network of electro-spun carbon fibers allows increasing the anode life [2]. Recently, paper-like membranes (PLMs) consisting of carbon fibers with embedded Ge-oxide nanoparticles (C/GeO₂) have been prepared via electro-spinning, followed by stabilization in air and carbonization in inert environment at moderate temperature (550 °C) in order to obtain high nitrogen contents, which improves the electrode wettability. The PLMs have been tested as binder- and collector-free anodes in flexible LIBs [1]. By varying Ge-load of the spinnable solution (38.5–65.4 wt% relative to the polymer) specific capacities in the range 400–600 mA h/g have been obtained, but with relatively poor stability.

This contribution presents results obtained by carrying out carbonization at higher temperatures (600–700 °C) in order to promote the co-formation of zero-valent germanium, which is known to play a catalytic role with beneficial effects on the reversibility of the Li⁺-insertion/extraction process [3].

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