FA.两岸三地新材料论坛

分会主席：王荣明、黄陟峰、郑子剑、阙郁伦

FA-01

Introduction to Nano-materials and Nano-devices Division of Chinese Materials Research Society (NND, C-MRS)

Rongming Wang

Beijing Key Laboratory for Magneto-Photoelectrical Composite and Interface Science, School of Mathematics and Physics, University of Science and Technology Beijing, Beijing 100083, China

The Nano-materials and Nano-devices Division, C-MRS (NND, C-MRS) is a non-profit, professional organization for materials researcher in the fields of nano-materials and nano-devices. Approved in Jan. 16, 2013, the founding conference of NND was held during April 26-28, 2014 in Suzhou, China. NND, as a secondary division of Chinese Materials Research Society, provides a collaborative environment for members on the idea exchange about the theoretical and applied investigations about the nanoscience. NND has held many international conference to promote the communication for the advancement of nanomaterials and nanodevices, including 2017 China-Japan-Korea Multifunctional Nanomaterials Seminar, the 3rd International Conference on Nanoenergy and Nanosystems, NENS2017, et. al.

FA-02

Chemical Synthesis and Theranostic Applications of Magnetic Iron Carbide Nanoparticles

Yanglong Hou, Jiali Hou, Hongchen Zhang, Yanmin Ju

College of Engineering, Peking University

With unique magnetic properties and feasible synthesis, magnetic nanoparticles (MNPs) have been widely used in cancer theranostics. Herein, we first introduce general protocle to produce monodisperse magnetic nanoparticles, and then highlight the synthetic process and theranostic applications of iron carbides, such as Fe_5C_2, Fe_2C, even multifunctional Au-Fe_2C nanoparticles (NPs). It' worth noting that the presence of halides is critical to produce pure phase iron carbides, while the growth thermodynamic and dynamic processes also affect the final products. In addition, through modification of affinity proteins ($Z_{HER2:342}$), Fe_5C_2 NPs can selectively bind to HER2 overexpressing cancer cells. T_2-weighted MRI and PAT signals are readily observed, and tumors are effectively ablated by PTT under NIR irradiation. Likewise, the $Z_{HER2:342}$-binding Au-Fe_2C NPs are capable of MRI/multispectral photoacoustic tomography/computed tomography tri-modal imaging-guided PTT. To enhance cancer therapeutic efficiency, anticancer drug doxorubicin is loaded into bovine serum albumin coated Fe_5C_2 NPs, combining PTT with chemotherapy. Such nanoplatform can respond to NIR and acidic environments, and exhibit burst drug release. In summary, we will present their chemical synthesis and application potential of multimodal imaging-guided PTT for precise diagnosis and efficient cancer treatment of iron carbide NPs.

Keywords: Magnetic Nanoparticles, chemical Synthesis, Theranostics, MRI

FA-03

Asymmetric Synthesis: the Methods and Applications

车顺爱

同济大学

FA-04

Oxide Heteroepitaxy for Soft Technology

Ying-Hao Chu

National Chiao Tung university

Soft technology has been an emerging field since flexible and wearable electronics started flourishing. In this research field, oxides can play an important role due to their intriguing functionalities and superior thermal and chemical stabilities. To deliver high-quality thin films or structures based on oxides, heteroepitaxy is essential. However, the lack of a suitable approach remains an obstacle for flexible oxide heteroepitaxy. Recently, due to the advancement of growth facilities and characterization tools, various

techniques are employed to acquire flexible oxide heteroepitaxy. This talk highlights the methods as well as direct and indirect approaches those are essential to develop oxide heteroepitaxy with mechanical flexibility. After that, I will provide an overview of classifying the fields in terms of applications where flexible oxide heteroepitaxy has been adopted and in particular, to develop oxide based approach.

FA-05

Adjustable thermal expansion in La(Fe, Si, Co)13/Cu conductive composites by high-pressure synthesis

Wei Wang[1,2], Laifeng Li[1,2]

1.School of Materials Science and Engineering, Tianjin University

2.State Key Laboratory of Technologies in Space Cryogenic Propellants, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences

Providing a suitable contact interface, where a high conductivity material with a proper coefficient of thermal expansion (CTE) adjoins the target semiconductor or thermoelectric devices, is very crucial to optimize the properties and service life of the relevant instruments. Regrettably, a high conductivity, low thermal expansion and relatively inexpensive material is very rare. Composites, fortunately, can offer the method to design and manufacture materials with adjustable properties by mixing two or more diverse constituents. In this paper, high conductivity composites with adjustable thermal expansion are successfully prepared by a moderate temperature high-pressure synthesis. The composites are based on combining La(Fe,Si)13-based compounds, the materials showing a giant, isotropic and nonhysteretic negative thermal expansion (NTE) properties, within Cu matrix. The La(Fe,Si)13-based compounds were used to adjust the CTE of the composites, while the Cu phase is in charge of tuning the thermal and electrical conductivity properties. Thus, by changing the relative amount of the two components, the composites with high conductivities and adjustable CTE were achieved. Furthermore, the thermal expansion and magnetic properties of composites are investigated by the physical property measurement system. The present results highlight the potential applications of the Cu-based high conductivity composites with room-temperature NTE properties in the thermal contacts to various semiconductor and microelectronic devices.

FA-06

Quantum Dots based Photocatalysts for Efficient Hydrogen Evolution

Tierui Zhang

Key Laboratory of Photochemical Conversion and Optoelectronic Materials/Technical Institute of Physics and Chemistry, CAS, Beijing, 10190, China

Quantum dots (QDs) have been paid much attention in the field of photocatalysis due to their excellent capacity of light absorption and proper electronic structure. Recently, in order to improve the photocatalytic H_2 evolution activity of QDs-based phtocatalysts, we studied the relationship between the structures and performance of photocatalysts in detail by adjusting their light absorbance, separation of electron-hole pairs, and surface/interface reactions of photocatalysts, achieving the rational design and synthesis of photocatalysts and their perfromance control.

FA-07

Excellent electronic properties and oxidation resistance of 2D group-III and group-IV monochalcogenides

Jijun Zhao

Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

Two-dimensional (2D) group-III and group-IV monochalcogenides have provided a versatile platform for nanoelectronics, optoelectronics, and clean energy. Using first-principles calculations, we systematically investigate the chemical, electronic, piezoelectric and photovoltaic properties of monolayer group-III and group-IV monochalcogenides and their lateral heterostructures. Our results reveal superior oxidation resistance of the group-III and group-IV monochalcogenide monolayers, with activation energies for the chemisorption of O_2 on the 2D sheets in the range of 3.02 ~ 3.20 eV and 1.26 ~ 1.60 eV, respectively. However, the defective group-III monochalcogenide monolayers with single chalcogen vacancy are vulnerable to O_2, showing small barriers of only 0.26 ~ 0.36 eV for an O2 chemisorption. Compared with pristine systems, Janus group-III monochalcogenide monolayers, including Ga_2SSe, Ga_2STe, Ga_2SeTe, In_2SSe, In_2STe, In_2SeTe, $GaInS_2$, $GaInSe_2$, and $GaInTe_2$, possess larger in-plane piezoelectric coefficients up to 8.47 pm/V and additional out-of-plane piezoelectric coefficients of 0.07 ~ 0.46 pm/V due to the broken mirror symmetry. We predict that monolayer group-III monochalcogenides by oxygen functionalization are promising 2D topological insulators with sizeable bulk gap up to 0.21 eV. Finally, we propose several lateral heterostructures constructed by group-III and group-IV monochalcogenide monolayers. Most of these heterojunctions belong to type II band alignment, which can prevent the recombination of electron-hole pairs. The electronic properties of these lateral heterostructures can be effectively tailored by the number of layers, leading to high power conversion efficiency of solar light over 20%. Our theoretical results shed light on the utilization of the group-III and group-IV monochalcogenide monolayers for the next-generation 2D electronics and optoelectronics with high performance and environmental stability.

FA-08

Extraordinarily Strong Interlayer Interaction and High-Electron-Mobility in 2D Layered PtX_2

Yang Chai
The Hong Kong Polytechnic University

The crystal structure and physical properties of two-dimensional transition metal dichalocogenides (TMDs) are substantially dependent on the filling of d orbitals of transition metal. While the properties of group-6 TMDs have been extensively investigated, the group-10 TMDs with the richest d electrons remain relatively unexplored. We present experimental and theoretical studies on a new member of group-10 TMD - platinum disulfide (PtS_2). The indirect bandgap of PtS_2 can be drastically tuned from 1.6 eV (monolayer) to 0.25 eV (bulk counterpart), and the interlayer mechanical coupling is almost isotropic. Such unusual electronic and vibrational properties in group-10 TMD can be understood as a result of strongly interlayer interaction from the pz orbital hybridization of S atoms. Our studies not only provide fundamental understanding of the effect of d-electron count on the interlayer interaction in TMDs, but also distinguish PtS_2 as a system with exceptionally electronic and vibrational properties.

Two-dimensional (2D) layered semiconductors are of great interest for the applications of future nanoelectronics due to their finite bandgap, ultrathin body, and the absence of dangling bond. It still remains a fundamental interest to discover a 2D materials with widely tunable bandgap, high mobility and good stability. In this work, we reveal a semiconductor-to-semimetal phase transition of 2D layered $PtSe_2$, which is only dependent on the number of layers, instead of external effects (pressure, strain or lithiation). Our few-layer $PtSe_2$ field-effect transistor shows high room-temperature mobility (~210 $cm2V^{-1}s^{-1}$) in a back-gated configuration on SiO_2/Si, comparable to that of BP. Bulk $PtSe_2$ device exhibits the metallic-like conductivity (6.64×10^5 S/m) even higher than graphite. The characteristics of widely tunable bandgap of $PtSe_2$ allows it to be effectively response to near-infrared light, in which the photo-responsivity is one order of magnitude larger than that of BP. Furthermore, our results showed that $PtSe_2$ has much better air-stability (over 1 year) than BP.

FA-09

Low-Temperature Growth of Transition Metal Dichalcogenides (TMDs) Layered Materials Toward Phase-Engineered Hybrid Films

Yu-Lun Chueh
National Tsinghua University

Novel condensed matter systems can be understood as new compositions of elements or old materials in new forms. According to the definition, various new condensed matter systems have been developed or are under development in the recent years. 2D layered materials, including graphene, transition metal dichalcogenides (TMDs) allow the scaling down to atomically thin thicknesses and possess unique physical properties under dimensionality confinement. Chemical vapor deposition (CVD) process is the most popular approach for all kind of 2D materials due to its high yield and quality. Nevertheless, the need for high temperature and the relatively long process time within each cycle hinders for commercial development in terms of production cost. However, the transfer procedure has become one of the major limitations of the overall performance.

In the first part of my talk, I will present several approaches, including laser irradiation assisted-selenization (LIAS) process, fast microwave annealing and plasms enhance selenization processes to grow different two-dimensional transition metal dichalcogenides materials on the arbitrary substrate in my lab. The detailed formation mechanisms, microstructures and physical performances as well as its applications in gas sensors, photodetectors and water splitting behaviors based on these two 2D materials were reported and investigated.

Keywords: Transition Metal Dichalcogenides, Chemical vapor deposition, including laser irradiation assisted-se

FA-10

石墨烯功能组装材料在能源与环境领域前沿应用的一些例子

曲良体
北京理工大学

由于其突出的电、热、机械特性，高比表面积及环境稳定性等，石墨烯引起了人们广泛的关注。石墨烯及其宏观结构的物理和化学特性依赖于其可控组装与功能化修饰，进而影响其特定应用。我们发展了新的方法和技术如限域组装等，实现不同维度功能石墨烯的制备，包括零维的石墨烯量子点，宏观一维的石墨烯纤维、二维的石墨烯膜和三维的石墨烯骨架结构等。基于这些维度限定的功能结构，他们在能源与环境领域表现出独特的应用潜能。例如，特殊处理的石墨烯可作为产电材料，一旦遇到湿气便自发产生电能；三维结构的石墨烯有序组装结构具有高效光热转化效能，在光热产生清洁水方面具有重要应用前景。本报告将呈现石墨烯功能组装材料在能源与环境领域前沿应用的一些例子。

关键词：石墨烯；制备；组装；产电；光热

FA-11

Recent Progress in Structural Nano Materials and Potentials for Lightweight Applications

吕坚
香港城市大学

FA-12

钠离子电池：从结构设计到性能优化

余彦
中国科学技术大学

在过去的几十年中，一方面锂离子电池已经广泛的被应用在便携式电子产品中。另一方面由于全球锂资源的匮乏和分布不均衡，研究人员对发展与锂离子电池具有相似电化学机理，但是价格更为低廉的钠离子电池寄予了更高的期望。然而由于 Na^+ 半径相比 Li^+大很多，Na^+反复的嵌入/脱出极易导致多次循环后电极的结构陷，从而引起容量的衰减。因此，探索合适的室温钠离子电池的正、负极材料是急需解决的关键问题。针对正极材料中具有 NASICON 结构的材料($Na_3V_2(PO_4)_3$；$NaTi_2(PO_4)_3$)，我们最早提出设计双碳层结构 NASICON 材料($NaV_2(PO_4)_3$; $NaTi_2(PO_4)_3$)，获得高倍率超长循环寿命钠离子电池。

在负极材料方面，合金储钠类材料(P 基，Sn 基)作为钠离子电池负极材料时，具有非常高的理论容量（2600 mAh/g）。然而，作为负极材料时，合金储钠类材料的主要问题在于体积效应和内阻对循环性能、倍率性能等关键指标的影响。此外，此类材料的电导率较低，作为电极时电池内阻也相应增加，高倍率放电性能下降。为了解决这一类材料由于体积膨胀以及纳米颗粒的团聚问题造成循环性能差的缺点。我们通过构筑一系列的中空、核/壳结构的微纳结构，实现稳定长循环寿命的高容量电极。

关键词：钠离子电池；储能材料；电极材料

FA-13

Cost-effective and Scalable Manufacturing of Metal-mesh Transparent Electrodes for Flexible Applications

Wendi Li
The University of Hong Kong Shenzhen Institute of Research and Innovation

Transparent conducting electrodes (TCEs) are key materials in optoelectronic devices such as displays, light-emitting diodes (LEDs), touchscreens, solar cells, and smart windows. For better performance of these devices, it is important to develop transparent electrodes with low sheet resistance while maintaining good optical transparency. Currently the dominant materials for TCEs are thin films of transparent oxides (TCOs) demonstrating reasonably good electronic performances, but film brittleness, low infrared transmittance and low abundance limit its suitability for many industrial applications. To overcome these limitations, recently there have been several new generation TCEs based on graphene, carbon nanotube, metal nanowire networks and metal mesh is introduced. These alternative TCEs demonstrate much better performance in terms of optical transparency, electrical conductivity and flexibility, however, materials and fabrication methods involved in its production are expensive and time-consuming which hinder its widespread commercial applications.

Over the past several years, we have developed cost-effective approaches for fabricating flexible transparent metal mesh electrodes via simple solution processed steps involving lithography, electroplating and thermal imprint transfer. Some of the techniques developed in this direction are being commercialized towards mass production. Generally, in our process, a prototype transparent flexible copper metal-mesh electrode can be fabricated using five simple steps including: (i) mesh pattern formation into the spincoated polymer resist on FTO glass by lithography; (ii) deposition of copper by electroplating inside the trenches to form a uniform Cu mesh; (iii) etching the resist to get the bare Cu mesh on glass substrate; (iv) imprint the bare Cu mesh into the polymer film by thermal imprinting process; and (v) separation of the polymer film from the FTO glass to transfer Cu mesh to a flexible polymer substrate in embedded form. Variations of this process have been developed to achieve the better capability for mass production, higher pattern resolution, and more versatile choices of materials. Record-high performance has been demonstrated on the transparent electrodes fabricated using our approach. Various applications are being developed and will also be introduced.

FA-14

2D Materials in Energy and Environmental Applications: Piezocatalysis and Water Splitting

Jyh-Ming Wu
Department of Materials Science Engineering, National Tsing Hua University, 101, Section 2, Kuang-Fu Road, Hsinchu, Taiwan 30013

The decomposition of organic pollutants serves as an increasing challenge in chemistry, and a major impact for environmental purification associated with industrial wastes. A variety of semiconductor photocatalysts have been utilized for the advanced oxidation process to generate the reactive oxygen species, by producing the hydroxyl (OH.) radical via the illumination of the UV light and the visible light, as it can oxidize the organic pollutants, a major remediation for environmental purification. This work, I will report that the non-centrosymmetric structure of the catalyzing material was applied by an external force, an electric field was therefore built up instantly inside the piezoelectric crystal due to its spontaneous polarization, which can efficiently separate the electron and hole pairs to trigger the catalyzing process for destroying the organic matters and producing radicals species in the dark. The non-centrosymmetric structure have been discovered in 2D materials such as, MoS_2, $MoSe_2$, and WS_2 etc.. The piezoelectric response in the odd number of layers in 2D material possess the uniquely piezo-catalyst effect by applying a mechanical deformation, which provides a great potential role in the energy and environmental applications without any lighting assistance.

FA-15

储能材料热力学调控与传感器研究

孙立贤
桂林电子科技大学

FA-16

Bio-Inspired Synthesis and Self-Assembly of Functional Materials

Shuhong Yu
Department of Chemistry, University of Science and Technology of China

There is a rich and long history of gaining inspiration from nature for the design of practical materials and systems. Biominerals are well-known composites of inorganic and organic materials in the form of fascinating shapes and high ordered structures, which exist in Nature, for example, pearl, oyster shells, corals, ivory, sea urchin spines, cuttlefish bone, limpet teeth, magnetic crystals in bacteria, and human bones, created by living organisms. During the past few decades, it has been one of the hottest research subjects in materials chemistry and its cutting-edge fields to explore new bio-inspired strategies for self-assembling or surface-assembling molecules or colloids to generate materials with controlled morphologies, unique structural specialty, and complexity. Although the properties of nanomaterials are frequently superior to those of their bulk counterparts, translating the unique characteristics of nanoscale components into macroscopic functional materials still remains a challenge.

This lecture will report our recent advances on bio-inspired synthesis of a family of inorganic micro-/nano- structural materials and their macroscopic scale assemblies, including bio-inspired molecule induced synthesis of micro-/nano-inorganic materials, bio-inspired interfacial assembly of macroscopic assemblies and functionalization. Especially, we will report our recent effort on how to realize the bulk production of synthetic nacre spanning all the length scales either by predesigned matrix-directed mineralization process or a bottom-up self-assembly process. These macroscopic nanoparticle assemblies are emerging as a new material system, showing enormous application potentials in diverse fields.

Keywords: bio-inspired synthesis, inorganic materials, nanoscale building blocks, self-assembly, application

FA-17

生物相容材料构建的细胞外纳米基质用于神经干细胞在有限使用生长因子条件下的增殖和分化

张世卿 [1,3]，孙鹏 [1]，陈晓玲 [2]，高琪 [2]，林凯莉 [1]，V. A. L. Roy[2]，张宏启 [1]，赖伟超 [2]，黄陟峰 [1]，翁建霖 [1,3]

1.香港浸会大学

2.香港城市大学

3.北京师范大学香港浸会大学联合国际学院

随着世界老龄化人口的快速增长，神经退行性疾病（ND）,包括阿尔茨海默病（AD）和帕金森病（PD）等，被认为是对人类健康最严重的威胁疾病之一。然而现有的 ND 药物治疗只能缓解患者的临床症状而不能治愈疾病，同时化学药物往往会导致严重的副作用，大分子的药物通常较难通过血脑屏障到达 ND 的病变部位发挥治疗作用。由于药理学治疗 ND 的局限性，2017 年全球最大的制药公司辉瑞公司宣布终止研发新的 ND 治疗药物，新型有效的治疗方法的开发显得尤其重要。由于 ND 的主要发病机制是神经元功能和/或结构的丧失，通过诱导神经干细胞（NSCs）增殖和分化产生具有功能性的神经元，进行神经元替代疗法成为近年来最有希望治愈 ND 的方法。但是神经干细胞在自然条件下的增殖和分化的能力十分有限，需要添加多种生长因子（GF）进行诱导。由于生长因子作用具有多靶点性，进行细胞替代治疗时，残留的生长因子在体内具有较高的致癌风险。因此，迫切需要制定新的方法来诱导 NSC 在无生长因子或替他化学添加剂的条件下进行高效的体外增殖和分化。因此，为了满足这种紧急的临床需求，我们利用斜角沉积技术（GLDA）首次研发了新型生物相容性无机材料堆积构成的细胞外纳米基质（iSECnMs），用于在使用最低限度生长因子的情况下，在体外高效的诱导神经干细胞增殖和分化。iSECnMs 可以通过其物理特性刺激多种细胞信号通路用于促进 NSCs 的增殖和分化为具有功能性的神经元。iSECnMs 在显著促进神经干细胞向神经细胞分化的同时，通过显著降低生长因子等其他化学添加剂的使用将致癌和炎症反应的风险降至最低，达到更高的生物安全性；并且可以通过改变材料的特性来达到定制细胞生化方向的目的，对干细胞的研究及未来的临床治疗具有重要的指导意义。

关键词：纳米基质；神经干细胞；生长因子

FA-18

Interface Engineering of Optoelectronic Devices Based on Graphene-Like Materials

Jianbin Xu

The Chinese University of Hong Kong

In this presentation, I would like to present our recent advances in preparation and characterization of high-quality graphene, two-dimensional (2D) layered transition metal dichalcogenide (TMD) materials, more specifically, MoS_2, $MoTe_2$, and WTe_2 WTe_2, and their hybrid combinations with graphene and black phosphorus (BP), as well as their related high-performance optoelectronic devices.

I will firstly introduce several approaches for growth of graphene and 2D semiconducting materials with large-scale and high crystallinity, and high throughput if possible. Secondly, I will demonstrate a few new reliable transfer and assemble as well as interface engineering techniques, which is of technical importance for the device fabrication with desired material quality and clean interfaces. Thirdly I will show several device configurations for photodetection and modulation as well as molecular sensing with high performance. Particularly I will give several examples, namely the high response speed and detectivity of sensitized graphene phototransistors from visible to mid-infrared spectral regions, modulators in THz frequency range, the molecular sensors based on Raman enhancement on WTe_2.

Thanks to the much improved mechanistic understanding at the interfaces, we have successfully devised the high-performance optoelectronic devices by significantly reducing the electrically detrimental species in the active regions, whilst by leveraging on electromagnetic interactions via hybrid layered material/photonic structures, we are able to demonstrate the high performance optoelectronic devices from visible to the infrared spectral regions and beyond.

Acknowledgement The work is in part supported by Research Grants Council of Hong Kong, particularly, via Grant Nos. AoE/P-02/12, 14207515, 14204616, and CUHK Group Research Scheme. The work described in this paper is also partially

supported by a grant from the University Grants Committee of the Hong Kong Special Administrative Region, China (Project No. AoE/P-03/08). I would like to thank the National Science Foundation of China for the support, particularly, via Grant No 61229401. This work is made possible in collaboration with Profs. Emma Pickwell-MacPherson, X. R. Wang, Q. Miao, Y. Shi, H. K. Tsang, Drs. X. M. Wang, X. Wan, K. Chen, Z. F. Chen, L. Ye, X. D. Liu, Mr. L. Tao, H. Li, H. Chen, et al.
Keywords: graphene, 2D materials, optoelectronics

FA-19

Engineering Atomic-size Spin Defects in Diamond for Quantum-Enhanced Biosensing

Zhiqin Chu
Department of Physics, The Chinese University of Hong Kong

The signature of life are dynamic, i.e., living cells constantly alter their phenotypes and create specific functions in response to both intracellular and extracellular environments. To this end, the development of advanced imaging and sensing tools becomes more and more crucial for cell biology and precision medicine nowadays. Quantum-enhanced sensors based on the spin-dependent photoluminescence of nitrogen-vacancy (NV) centers in diamond offer great potential to achieve single-molecule detection with atomic resolution under ambient conditions. The NV centers are optically accessible with high spatiotemporal resolution, and have sharp magnetic resonances being sensitive to local change of magnetic field, temperature, force and rotation. In this talk, I will give an overview of quantum sensing based on NV centers, and present our studies of their usage towards biomedical science through interdisciplinary approaches. The unique quantum features of NV centers in diamond, together with their excellent biocompatibility and extraordinary long-term working capability, may lead to a number of excitements in biological and medical sciences ranging from measurements of temperature, pH, ion concentrations, free radicals, mechanical forces, to imaging magnetite biominerals associated with neurodegeneration, with unprecedented sensitivity and precision.

FA-20

Growth and physical property of semiconductor nanowires

Yi-Chia Chou
National Chiao Tung University

Many electronic devices, such as field-effect transistors, depend on achieving precise control of both the composition and atomic arrangement within a semiconductor nanostructure and the contact of the nanostructure with the larger-scale circuit. Here we show how complex nanostructures can be formed that include silicide and germanide nanocrystals embedded within Si and Ge nanowires. We form the silicide or germanide by adding the appropriate metal to the liquid droplets of VLS grown nanowires. Solid silicide or germanide nanocrystals form in the liquid and have freedom to move and rotate until a low-energy interface with the nanowire is found. After contact is made, certain types of silicide and germanide nanocrystals remain attached to the nanowire while others break away without forming a permanent contact. Only the nanocrystals that remain attached to the nanowire can then be incorporated by continued growth of the nanowire. We have examined the factors that determine crystal adhesion to the nanowire and suggest that it depends on the symmetry of the contact interface and hence the crystal structures of the materials. To expand the range of possible materials, we introduce the use of phase transformations within the nanocrystal. The variety of nanostructures with incorporated nanocrystals that it is possible to make using such reaction schemes potentially raises the chances for designing particular electronic and contact properties for nanostructured device applications.
Keywords: Nanowires

FA-21

Novel Functional Dendritic Polymer Materials

Ken Cham-Fai Leung
Department of Chemistry, The Hong Kong Baptist University, Kowloon Tong, Kowloon, Hong Kong SAR

Type III-B rotaxane dendrimers (T3B-RDs) are hyperbranched macromolecules with mechanical bonds on every branching unit. Here we demonstrate the design, synthesis, and characterization of first to third (G1–G3), and up to the fourth (G4) generation (MW > 22,000Da) of pure organic T3B-RDs and dendrons through the copper-catalyzed alkyne–azide cycloaddition (CuAAC) reaction. By

utilizing multiple molecular shuttling of the mechanical bonds within the sphere-like macromolecule, a collective three-dimensional contract-extend molecular motion is demonstrated by diffusion ordered spectroscopy (DOSY) and atomic force microscopy (AFM). The discrete T3B-RDs are further observed and characterized by AFM, dynamic light scattering (DLS), and mass spectrometry (MS). The binding of chlorambucil, a drug for leukemia treatment, and pH-triggered switching of the T3B-RDs are also characterized by NMR spectroscopy.

Keywords: Polymer, dendrimer, supramolecular chemistry, drug delivery

FA-22

Design and Preparation of High Energy Density Dielectric Capacitors: From bulk to thin film

林元华
清华大学

Developing high-performance film dielectrics for capacitive energy storage has been a great challenge for modern electrical devices. Exploring dielectric capacitors with high energy density, i.e., high dielectric permittivity, high breakdown electric field, and low dielectric loss, has recently aroused considerable interest. We designed a sandwich-structured PVDF-based composite film with both of BSBT-nf and TO-np as the nano fillers fabricated by a layer-by-layer casting process, and obtained a high energy density ~20 J cm^{-3} is achieved at 646 kV mm^{-1}. Recently, we demonstrate that giant energy densities of ~ 70 J cm^{-3}, together with high efficiency as well as excellent cycling and thermal stability can be achieved in the lead-free $BiFeO_3$-$SrTiO_3$ solid-solution films through domain engineering. It is revealed that the $SrTiO_3$ incorporation can transform the ferroelectric micro-domains of $BiFeO_3$ into highly-dynamic polar nano-regions, resulting in a ferroelectric to relaxor-ferroelectric transition with concurrently improved energy density and efficiency.

FA-23

Progress and Prospects of GaN-based VCSEL from Near UV to Green Emission

Haochung Kuo
National Chiao Tung University

GaN is a great material for making optoelectronic devices in the blue, blue-violet and green. Vertical-cavity surface-emitting lasers (VCSELs) have many advantages such as small footprint, circular symmetry of output beam, two-dimensional scalability and/or addressability, surface-mount packaging, good price-performance ratio, and simple optics/alignment for output coupling. In this paper, we would like to (1) review design of GaN-based VCSEL-include some challenges; (2) design and MOCVD growth of electrically pumping blue VCSEL; (3) world first Green VCSEL using QD active region to overcome the green gap; (4) Novel GaN-based VCSEL using high-contrast-grating (HCG) reflector. Finally GaN VCSEL for visible light communication

Keywords: Vertical-cavity surface-emitting lasers; GaN; visible light communication

FA-24

Polar and Nonpolar ZnO Nanostructured Films for Functional Sensor Devices

Da-Hua Wei
Institute of Manufacturing Technology, National Taipei University of Technology (TAIPEI TECH)

Anisotropy is a distinctive property in crystalline structure. Every dissimilar crystal facets or surfaces have different geometric electronic structure and atomic arrangement resulting in various functional properties. Basically, wurtzite-structure ZnO crystal tends to grow polar {0001} direction along the *c*-axis due to the strongest anisotropy in the growth rate, which has attracted a significant amount of attention and has been employed in many application fields. Perpendicular to the *c*-axis, the nonpolar {10-10} and {2-1-10} direction of ZnO are other crystal facet which have also been extensively studied owing to absence of spontaneous polarization in crystal and with an equal number of oxygen and zinc ions on the surface. Therefore, the purpose of presented work is to investigate the fabrication and characterization of polar and non-polar ZnO thin films and the performance of polar and non-polar ZnO thin film employed in UV photoconductive devices. It is worth mentioning that studies of nonpolar ZnO thin film toward UV photodetector are still under development in research fields. Experimentally, our group used plasma enhanced chemical vapor deposition (PECVD) system to synthesize polar and non-polar ZnO thin films. After below systematic investigated characterizations including X-ray diffraction (XRD), optical emission spectroscopy (OES), field emission scanning electron microscope (FE-SEM), atomic force microscope (AFM), and photoluminescence (PL), the polar and non-polar ZnO thin films synthesized onto silicon substrates have been successfully demonstrated. The high quality polar (0002) plane ZnO thin film was synthesized under growth temperature of 350 ^{o}C, while the non-polar ZnO thin film combined with (10-10) and (11-20) planes was synthesized at 550 ^{o}C. In order to fabricate the UV photoconductive devices, the interdigitated platinum (Pt) contact electrode was prepared onto ZnO thin films by conventional optical lithography process and radio frequency magnetron sputtering. The as-fabricated devices were annealed in argon circumstance by rapid thermal annealing (RTA) for obtaining Ohmic contact between the electrodes and the ZnO films. The responsivity, reliability, and response time of the polar and non-polar ZnO thin film UV photoconductive devices were tested by current-voltage (*I-V*) curve of photo and dark current and time-dependent photocurrent measurement, respectively. Both polar and non-polar detectors showed a prominent photocurrent gain under UV light illumination, compared with dark conditions. However, the response and recovery times for the non-polar detectors were significantly faster compared to the polar detectors.

FA-25

新型二维磁性 CrO_X 与 Cr_2C 半导体材料的第一性原理研究

孙志梅

北京航空航天大学

基于铁磁半导体的自旋电子器件，如非易失磁存储器，具有功耗低、操作速度快、存储密度高和数据保持力强等优势，且可望将存储和计算融为一体，在未来信息技术和量子计算等领域具有广阔的应用前景。二维磁性半导体材料对提高自旋电子器件性能至关重要，然而，大多数二维材料，包括石墨烯等，都不具有本征铁磁性，需要通过掺杂改性等方法引入磁性。因此，寻找高居里温度的新型二维磁性半导体将为自旋电子器件的研究提供重要基础。本报告将阐述近期我们在二维磁性半导体材料方面的研究进展，主要包括以下两方面的内容。（1）通过第一性原理计算和第一性原理分子动力学模拟等方法，我们提出了一种获取二维本征铁磁半导体的新途径，即通过剥离反铁磁的范德瓦尔斯半导体获得单层铁磁半导体；并预测了一类新型二维本征铁磁半导体——单层 CrOCl 和 CrOBr 材料，其居里温度远高于文献报道的二维 CrI_3 和 $Cr_2Ge_2Te_6$。计算结果表明，该系列二维材料可以采用类似制备石墨烯的机械剥离法获得，具有良好的动力学和热力学稳定性。该工作为发展新型二维本征铁磁体提供了新思路，所预测的二维铁磁 CrOCl 和 CrOBr 材料有望应用于未来自旋电子器件。（2）半金属铁磁性二维 Cr_2C 晶体的预测及其表面功能化诱导的金属-绝缘体相变。基于杂化泛函密度理论，我们在 MXene 家族中预测了第一个半金属铁磁体材料，且具有可调的电子性质和磁性的 Cr_2C，其电荷输运完全由自旋向上的电子所主导，即通过 Cr_2C 的电子流将是 100%自旋极化的。Cr_2C 的半金属带隙高达 2.85 eV，保证了这一 100%自旋过滤特性可以在一个大的偏压范围内应用。当 Cr_2C 的表面被 F、OH、H 或者 Cl 原子基团饱和后，Cr_2C 将经历从金属到绝缘体的转变，同时伴随铁磁到反铁磁的转变。因此，通过控制表面功能化原子基团种类，可以很好地控制反铁磁态的能隙宽度。

关键词：磁性半导体；第一性原理计算；二维材料

FA-26

Ambipolar Organic Field-effect Transistors based on Dual-function, Ultra-thin and Highly Crystallized 2,9-didecyldinaphtho[2,3-b:2, 3-f]thieno[3,2-b]thiophene (C10-DNTT) Layer

Paddy K.L Chan

Department of Mechanical Engineering. The University of Hong Kong, Hong Kong

We utilize a novel dual solution shearing method to deposit single-crystallized and densely packed ultra-thin 2,9-didecyldinaphtho[2,3-b:2, 3-f]thieno[3,2-b]thiophene (C10-DNTT) films. We further converted this C10-DNTT layer to ambipolar OFET applications. We demonstrated the C10-DNTT can not only be used as the p-type channel in a bilayer OFET device but also as a growth template of the upper n-type channel and in our case we used Copper(II) 1,2,3,4,8,9,10,11,15,16,17,18,22,23,24,25-hexadecafluoro-29H,31H-phthalocyanine (F16CuPc) layer. The C10-DNTT molecules with long and closely packed alkyl chains in function as a self-assembly monolayer(SAM) to assist the ordered orientation F16CuPc. The drain-source current (IDS) in the hole channel and n-channel show a 3-fold and 5-fold increase compare with two-step thermal evaporation, which can be attributed to more efficient charge transfer and higher crystallinity of the organic semiconductor crystals. Our findings demonstrate solution-processed ultra-thin single-crystallized organic thin films can be a promising candidate in multi-layer organic electronics. In this talk, we will further explore the potential of single crystals template fabricated by physical vapor transport (PVT) method. We study the charge transfer and ambipolar properties of bilayer thin films constructing by PVT processed rubrene singe crystals and F16CuPc through electrical and crystallographic and topographical characterizations.

FA-27

Smart Materials and Devices Driven by a Metal-Insulator Phase Transition

Kai Liu

Tsinghua University

Various mechanisms are currently exploited to transduce a wide range of stimulating energies into mechanical motion. At the microscale, simultaneously high amplitude, high work output, and high speed in actuation are hindered by limitations of these actuation mechanisms.VO_2 is a strong-correlated oxide that undergoes a thermally driven metal−insulator phase transition (MIT) accompanied by a structural transition slightly above room temperature (68 °C). As its lattice changes from monoclinic (insulating, I) to rutile (metallic, M) structure upon heating across the MIT, VO_2 shrinks by a transformation strain of $\varepsilon \sim 1\%$ along the c-axis of the rutile phase while expanding along the other two directions. This structural transition delivers high-performance microscale actuations that convert energy from light, heat, or electricity into mechanical motion. Designed to bend, flex, flap, or oscillate when energized, they can become the motors, switches, pumps, and valves of microfluidic systems. Fashioned into coils, they can rotate as fast as 200,000 rpm without breaking. Such microscopic bending and torsional machines could become the mechanical building blocks in the applications of robotics, artificial muscles, smart windows, and drug delivery.

Keywords: actuator; phase transition; carbon nanotube; vanadium dioxide; smart device

FA-28

稀土离子掺杂玻璃上转换发光特性

肖志松，刘佳铭，黄馨

北京航空航天大学

稀土离子因其特殊的电子层结构，使其内部 4f 组态内的跃迁发光不受周围环境的影响，发光波长可覆盖从可见光到中红外的波长范围。稀土离子掺杂的发光玻璃在显示、光通信、光学放大以及固体激光器等领域都有广泛的应用。虽然氟化物玻璃声子能量低，透过窗口宽，是优良的发光基质材料，但其制备复杂、化学和物理性能较差，热稳定性不如氧化物玻璃，较难拉制光纤，因而在实际应用上受到一些限制。氟碲酸盐玻璃，通过调整组分和工艺，简化了制备过程，并且结合了氟化物玻璃声子能量低，碲酸盐玻璃化学稳定性和机械性能好的优势，能有效的提高稀土离子发光强度。通过合理设计配比，采用传统的熔融法，制备了一系列不同浓度的稀土离子掺杂氟碲酸盐玻璃，得到了一系列具有优良上转换发光性能的样品，在光学温度传感和 LED 等方面具有良好的应用前景。

关键词：稀土；光学温度传感；LED

FA-29

Photoelectrochemical and self-powered ZnO/Cu_2O biosensor

Hsiangchen Wang

National Chung Cheng University

Any common current sensor requires an extra bias voltage. However, the measuring mode may interfere with the actual measurements. To provide an extra bias voltage originally required for detection, a current sensor must be self-powered. The simplest structure for this purpose is a p-n junction photodiode coupled with a simple photoelectric performance analyzer or an electrochemical analyzer for electrical measurement. The p-n heterojunction photoelectrochemical biosensor, which comprises a p-type Cu_2O film formed by electrochemical deposition and n-type ZnO nanorods formed by the hydrothermal method, is prone to photoelectrochemical reactions and self-powered. Four types of human esophageal cancer cells (ECCs) were detected by this biosensor without requiring an extra bias voltage. The measured photocurrent values of high invasion capacity cancer cells was consistently 2 times higher than those measured by a slight invasion capacity cancer cells. The response time, which was about 0.5 s, allowed repeated measurement.

Keywords: photoelectrochemical biosensor, Cu_2O, ZnO, esophageal cancer cells

FA-30

功能材料的纳米力学行为

陆洋，张洪题
香港城市大学

作为最重要的半导体材料，硅晶体宏观状态下坚硬且脆。但是作为纳米电子器件中最重要的一维纳米材料，如果硅纳米线能够实现超大弹性将会对其在柔性器件中的应用具有重大的意义。在本工作中，我们发现了使用气相化学沉积方法制备的直径在 100 纳米左右的单晶硅纳米线在室温下能够被拉伸到超过 10%的可回复弹性应变。其中一些样品的弹性拉伸应变值更是达到了 16%，接近了其 17-20%的理论弹性极限值。我们进一步通过在不同应变速率的循环加载卸载实验证明了硅纳米线的超弹性形变过程是完全可回复的，并且其相应的应力应变曲线没有出现明显的回滞现象，断裂后的形貌也没有任何塑性变形迹象。通过进一步对其断裂行为的分析研究，我们论证了硅纳米线在这种超大弹性下依然是典型的脆性断裂，且之所以能够达到此种特性要归结于其纳米级别的尺寸、原始无缺陷的单晶晶体结构以及原子级别光滑的表面。我们的工作预示着其他半导体纳米线也可能有类似超弹性形变特性，并且该特性会使其在柔性电子以及纳米生物界面等多种前沿领域中的应用成为现实。此外，超弹性形变过程中晶格的巨大畸变所导致的带隙结构变化会对新兴的“弹性应变工程”领域有着巨大的潜力。

FA-31

Application of Modern TEM on Novel Functional Materials

Ye Zhu[1], M. U. Rothmann[2], W. Li[2], U. Bach[2], Y.-B. Cheng[2], J. Etheridge[2], X.B. Cai[3], X. Gao[4], G. Liu[4], A. Tricoli[4], N. Wang[3]
1.Department of Applied Physics, The Hong Kong Polytechnic University
2.Department of Materials Science and Engineering, Monash University
3.Department of Physics, Hong Kong University of Science and Technology
4.Nanotechnology Research Laboratory, Research School of Engineering, Australian National University

Materials science relies on understanding and manipulating structure-property relationship at the nano- and atomic level. Owing to the unmatched spatial resolution, transmission electron microscopy (TEM) has become an indispensable tool to elucidate material structure. The advent of aberration correctors has further improved the resolution of TEM to the unprecedented sub-angstrom level, leading to groundbreaking discoveries including imaging oxygen octahedral tilting in complex oxides and mapping electric polarization in ferroelectrics.

In this talk, I will discuss our recent results using TEM to advance the understanding of novel material structure as well as the associated functionalities. By carefully controlling the electron dose, we first derived the damage mechanism in perovskite $CH_3NH_3PbI_3$ under an electron beam, which helps to recognize the artefacts of TEM imaging on this important but beam-sensitive material. Furthermore, we developed a low-dose imaging condition that can reliably characterize the pristine structure of $CH_3NH_3PbI_3$ in TEM. Using this imaging condition, we successfully revealed the ferroelastic twinning structure intrinsic to $CH_3NH_3PbI_3$, which forms during cubic-to-tetragonal structure transition under cooling.

In another example, we used atomic-scale electron energy-loss spectroscopy (EELS) to identify the configuration of Ce dopants in Mn_3O_4 nanocatalysts. We discovered solitary Ce dopants as well as nanoclusters, both inside nanocatalysts and at the surfaces. The different phases of Ce dopants can convert to each other, providing an effective oxygen-storage/release route that is responsible for the enhanced redox catalytic activity from Ce doping.

Keywords: TEM; EELS; $CH_3NH_3PbI_3$ perovskite; twin; Mn_3O_4 nano-catalysts

FA-32

Designing Nano-Arrays for SERS-based Rapid Detection of Trace POPs

Guowen Meng, Zhulin Huang, Chuhong Zhu, Haibin Tang
Institute of solid state physics, Chinese Academy of Sciences

Persistent Organic Pollutants (POPs) pose a big threat to human beings and the environment. POPs are highly toxic and persistent, and can travel long distance in the environment and bio-amplify through the food-chains, so even small exposures may eventually reach dangerous levels. Traditional techniques for detecting POPs include gas chromatography, immunoassays, ion detection technique, and high-resolution mass spectrometry. However, these large-scale sophisticated analytical instruments are usually used in centralized laboratories, and not suitable for real-time field-deployable detection. Therefore low cost rapid detection of trace-level POPs is extremely important.

Surface-enhanced Raman scattering/spectroscopy (SERS) is a powerful tool for rapid identification of analytes with high sensitivity and fingerprint characteristics. Therefore SERS has potentials in rapid detection of trace POPs. One of the key issues in SERS-based detection is the building of effective substrates with enough SERS "hot spots" to ensure both high sensitivity and excellent SERS signal reproducibility. As highly ordered noble metal nano-arrays usually contain uniformly distributed nano-gaps, sharp-tips/edges, which may produce highly concentrated electromagnetic fields associated with strong localized surface plasmon resonance so that SERS "hot spots" will occur at these positions. On the other hand some semiconductors have chemical supporting Raman enhancement. Based on these points of view we have built various metal/semiconductor nano-arrays with remarkable SERS sensitivity and signal reproducibility for various POPs, paving the way to the SERS-based rapid field-deployable detection of trace-level POPs.

Keywords: Nanostructures, Surface enhanced Raman Scattering spectroscopy, rapid detection, Trace-level, POPs

FA-33

Phase Transition and Solid Refrigeration Materials

Fengxia Hu

Institute of Physics, Chinese Academy of Sciences

Solid refrigeration technology based on giant magnetocaloric and barocaloric effect has attracted world-wide attention due to the numerous advantages over vapor compression refrigeration which have low efficiencies and negative environmental effects. The coupling of magnetic and structural transition, i.e. magnetostructural transition, is usually sensitive to magnetic field and stress, thereby leading to giant magnetocaloric effect (MCE) and barocaloric effect (BCE).

Here we report stress modulated phase transition and multi-field driven magnetocaloric effect for the well-known $La(Fe,Si)_{13}$ materials, as well as the MM'X materials. Enhanced mechanical properties and age stability have been achieved in the hydrogenated $La(Fe,Si)_{13}Hd$ plates as thin as 0.4~0.6mm with extra Fe. MnCoGe-based alloys with magnetostructural transition show giant negative thermal expansion behavior and MCE, but the bad mechanical properties obstruct their practical applications. We successfully grew Mn-Co-Ge-In films on different substrate, which completely overcome the breakable nature and tunable MCE around room temperature has been observed owing to the stress from substrate. For the FeRh/PMN-PT and $LaPrCaMnO_3$/PMN-PT heterostructures with distinct magnetic properties, a significant reduction of hysteresis loss and a tunable MCE has been achieved by utilizing the stress generated by electric field. Moreover, we also studied stress modulated spin orientation in a number of heavy rare earth (R)-based compounds. Spin orientation is usually accompanied by a change of lattice symmetry. Pressure modulated and enhanced MCE has been demonstrated in RGa and RCo_2 compounds. For example, in PrGa, hydrostatic pressure can largely shift the spin reorientation temperature because of the significant change of lattice parameter along with the spin reorientation. Although the maximum entropy change ΔS decreases with pressure, an asymmetric broadening of ΔS with magnetic field occurs due to the widening of metamagnetic transition caused by pressure. As a result, a plateau develops on the ΔS-T curve, and 10% improvement of effective refrigerant capacity RCeff has been achieved. Analysis indicates that the origin can be closely relative to the significant impact of the pressure on the crystal field interaction.

Keywords: Phase transition, solid refrigeration materials

FA-34

Optical management of solution-processed silicon-nanowire based optoelectronic devices

Chia-Yun Chen

Department of Materials Science and Engineering, National Cheng Kung University

Solution-processed technologies are promising for the development of next-generation optoelectronic devices owing to the potential for low-cost fabrication. In this study, the employment of shape-controlled silicon nanostructures for the construction of low-cost photovoltaic cells was explored with three specific strategies: (1) Optimization of light-trapping effect, (2) interface management and (3) improvement of UV absorption. The impacts of formed silicon nanostructures on the photovoltaic performances of solar cells were revealed, indicating that the efficiency of nanostructure-based hybrid solar cells could be improved by reducing the defective sites essentially arisen from the contact non-uniformities at the interfaces of heterojunction. Such hybrid designs exhibited the improved conversion efficiency with 3.3 times greater than that of untexturized devices. We anticipate that our results will be a starting point for the understanding of nanostructured silicon for the practical photovoltaic devices, and further benefit the development of photocatalytic and photodetection applications.

FA-35

Semiconductor Nanoheterostructures for Photoconversion Applications

Yung-Jung Hsu
National Chiao Tung University

With the inherently high degree of complexity, nanoheterostructures composed of two or more materials joined in unique architectures may exhibit superior synergetic properties that are difficult or impossible to acquire from their individual constituents. For semiconductor nanoheterostructures, the relative band alignment of the constituents promotes effective charge separation to bring them desirable properties for photoconversion applications. Several representative works from our lab including Au-CdS, Au-ZnS core-shell nanocrystals, Cu^{2+}-doped ZnO nanocrystals, graphene quantum dot-modified CdSe nanocrystals, and Au@Cu_7S_4-decorated TiO_2 nanowires will be introduced to demonstrate the promising potentials of semiconductor nanoheterostructures.

FA-36

Upconversion-based All-optical Optogenetics

Peng Shi
City University of Hong Kong

Many nanomaterials can be used as sensors or transducers in biomedical research and they form the essential components of transformative novel biotechnologies. In this study, we present an all-optical method for tetherless remote control of neural activity using fully implantable micro-devices based on upconversion technology. Upconversion nanoparticles (UCNPs) were used as transducers to convert near-infrared (NIR) energy to visible light in order to stimulate neurons expressing different opsin proteins. In our setup, UCNPs were packaged in a glass micro-optrode to form an implantable device with superb long-term biocompatibility. We showed that remotely applied NIR illumination is able to reliably trigger spiking activity in rat brains. In combination with a robotic laser projection system, the upconversion-based tetherless neural stimulation technique was implemented to modulate brain activity in various regions, including the striatum, ventral tegmental area, and visual cortex. Using this system, we were able to achieve behavioral conditioning in freely moving animals. Notably, our microscale device was at least one order of magnitude smaller in size (~100 µm in diameter) and two orders of magnitude lighter in weight (less than 1 mg) than existing wireless optogenetic devices based on light-emitting diodes. This feature allows simultaneous implantation of multiple UCNP-optrodes to achieve modulation of brain function to control complex animal behavior. We believe that this technology not only represents a novel practical application of upconversion nanomaterials, but also opens up new possibilities for remote control of neural activity in the brains of behaving animals.

Keywords: upconversion materials, neural stimulation, near-infrared light, remote control, wireless optogenetics

FA-37

Solution Process Organic Semiconductors in Printable Solar Photovoltaic Devices

Gang Li
Department of Electronic and Information Engineering, The Hong Kong Polytechnic University

Solar energy provides limitless resource for human being to address the terawatt energy challenge. The ideal photovoltaic (PV) technology needs to be earth abundant, non-toxic, and very low cost etc. Scientists have long dreamed of printing solar cells like newspaper, and can apply to any surface to generate electricity.

Solution processed solar cell based on organic polymer (Macromolecule) and organometal halide hybrid perovskites are both promising candidates for printable PV technologies. The advantages include low material cost, low temperature fabrication and their compatibility with printing/coating processes (roll-to-roll), high material utilization etc. They also provide attractive properties like flexibility, light weight, and transparency.

This talk will first cover some of key progresses in solution processed polymer solar cells: (a) Morphology control and understanding; (b) Organic semiconductor/electrode interfaces; and (c) Device architecture investigation (inverted architecture, inverted tandem polymer solar cell) for high performance OPV with over 11% efficiency.

Recent works on organometal halide perovskite optoelectronic devices will be discussed, focusing on interface engineering and the devices incorporating organic semiconducting polymers and small molecules. We incorporated OPV donor polymer and non-fullerene acceptor into the anti-solvent for perovskite film formation process, through which higher efficiency and much enhanced solar cell stability was achieved – storage, thermal as well as light illumination stability.

The R&D challenges & opportunities on printable solution process solar cell as viable PV technology will be discussed.

Keywords: Solution Process, Organic Semiconductors, Polymer solar cells, Perovskite solar cells

FA-38

The Multi-scale Structured Anode Materials for Lithium Ion Batteries

Min Zhu

1.School of Materials Science and Engineering, South China University of Technology

2.Guangdong Provincial Key Laboratory of Advanced Energy Storage Materials

Various methods of energy convert and store have been developed and widely used as power sources for applications in various portable electronic devices, and electric vehicles. Lithium ion batteries have been intensively studied due to their high energy density and high specific power. However, there are still big challenges for the further development of high performance rechargeable lithium ion batteries. One of the main challenge for the anode materials of lithium ion battery is the conflict between high capacity and cycleabilitiy(reversibility).

In our studies, multiscale structure has been designed and created in Sn based materials with the emphasis on overcoming the stress-strain effects due to the charge/discharge of high amount of lithium in the high capacity electrode materials, as well as on the mechanism of interaction among different active phases. The interface effects on Li storage capacity, cyclability and Li diffusion kinetics of the materials have also been investigated. In our studies, Sn based Li storage materials with multi-scale structure have been successfully prepared by evaporating/sputtering deposition, plasma assisted milling and nanocapsulating. It has been found that the multi-scale and multi-phase structure help to achieve high Li storage capacity, long cycle life and good high-rate capability in the Sn-based anodes.

Based on our studies, it is believed that manipulating the multi-scale and multi-phase structures offers an important means of further improving the capacity and cyclability of metal-based materials for Li storage.

Keywords: Lithium ion battery; Anode; Multi-scale structure

FA-39

Construction of Carbon Interface for Electrical Energy Storage

Yanwu Zhu

1.Department of Materials Science and Engineering, USTC

2.Key Laboratory of Materials for Energy Conversion, Chinese Academy of Sciences

Graphene and related materials have attracted much attention in the fields electric energy storage. For the practical application in energy storage devices, tailoring the 3D carbon architectures is critical for achieving the comprehensively useful performance of the devices. In addition, constructing the carbon interface and understanding the interface is essential to further improve the performance. Herein our recent progress will be included in the talk, mainly focusing on the approach combining self-assembly and chemical processing developed for high volumetric performance of supercapacitor electrodes, high rate Li-ion battery electrodes and novel carbon monoliths with potentially new physical properties. Also, some recent progressing on the interface mechanisms towards understanding the kinetics of ions between graphene layers and probing the Li-ion deposition on single layer graphene will be discussed, based on ex-situ and in-operando techniques.

Keywords: carbon electrode, electrochemistry, interface

FA-40

Nanoscale p- and n-type Field-Effect Devices of P3HT and ZTO Nanowires

Wen-Bin Jian, Jian-Jhong Lai, Bo-Rui Feng

Department of Electrophysics, National Chiao Tung University

The nanowires based field-effect transistors attract a great attention since the exploration of devices on the nanoscale helps to clarify physical mechanisms. Reasoning of the nanoscale mechanisms facilitates structural designs of large-scale field-effect transistors and photovoltaic cells. Poly(3-hexylthiophene-2,5-diyl) (P3HT) nanowires have a size of about 10 nm while several microns in length. They are ideal nanowires to make a nanoscale contact on other nanowires. Most importantly, P3HT nanowires are intrinsically p-type semiconductors. On the other hand, zinc tin oxide (ZTO) nanowires present an intrinsically n-type behavior. The average diameter of ZTO nanowires is about 100 nm. In our previous report, we have studied the interplay of hybrid P3HT/ZTO interface on optoelectronics and photovoltaic cells [1]. Here, we report the device performance and the transfer characteristics of the P3HT nanowire, the ZTO nanowire, and the nanoscale pn devices. We focus on the on-off ratio, the mobility, the on and the off currents. The mobility of the p-type P3HT nanowires is about 10-4 cm2/V s which is about one thousandth of the largest value reported in the literature. In contrast, the mobility of the n-type ZTO nanowires is about 0.1 cm2/V s. The large difference in mobility between the P3HT and ZTO nanowires will affect the nanoscale pn junction, the light induced photocurrents, and the photovoltaic properties.
Keywords: P3HT nanowires; ZTO nanowires; nanoscale field-effect transistors; photocurrents; photovoltaic cells

FA-41

Two-Dimensional Metal Chalcogenide Semiconductors: Design, Synthesis and Applications

Jun He
National Center for Nanoscience and Technology, Beijing

While scaling the dimension(s) of semiconductors down to nanoscale, novel properties, such as ultrahigh specific surfaces and strong electrostatic tunability, will show out. Among the various low dimensional structures, two-dimensional (2D) semiconductors may lead the next generation of electronics and optoelectronics due to their compatibility with traditional micro-fabrication techniques and flexible substrates. Up to now, both layered and non-layered materials have been demonstrated to present in 2D geometry. As for the former, even though big breakthroughs, especially on transition metal dichalcogenides (TMDCs), have been made, more systematical and deeper studies are needed. In addition, inspired by the success of 2D layered materials and the fact that many materials with significant functions have non-layered crystal structures, 2D non-layered materials have attracted increasing attentions. Based on above challenges and motivations, our research focuses on the design, synthesis and applications of low dimensional metal chalcogenides semiconductors. In this talk, I will present our recent progress on the following two aspects:

(1) 2D layered metal chalcogenide semiconductors: controllable synthesis, properties, electronic and optoelectronic applications.

(2) Van der Waals epitaxial growth, electronic and optoelectronic properties of 2D non-layered materials, such as CdTe, Te and Pb1-xSnxSe nanosheets.

Keywords: 2D layered materials, 2D non-layered materials, Van der Waals epitaxial growth, electronic and optoelectronic applications

FA-42

Ferroelectric domain wall memory in hierarchical domain pattern and huge readout wall current

Anquan Jiang, Zilong Bai, Dongfang Chen
Fudan University

The conductive domain walls in an insulating ferroelectric matrix offer the potential to read out the various polarization states for mass data storage. The 71°, 109° and 180° domain walls with atomic thickness in multiferroic $BiFeO_3$ (BFO) thin films have been found to be conductive with wall currents on the order of pA-nA, insufficient to enable high-speed sense amplifiers to read the stored information, because the Johnson-Nyquist limitation revealed that a current of at least 0.1 mA was necessary for a read time of 10 ns.

Here we fabricated epitaxial BFO films through pulsed laser deposition on (001) $SrTiO_3$, (110) $GaScO_3$, and (110) $SrTiO_3$ substrates using a KrF excimer laser with an operating wavelength of 248 nm. Films with thicknesses of between 35 nm and 120 nm were grown at an optimized substrate temperature of 602°C. After film growth, the top electrode patterns were then formed by electron beam lithography. The film morphology was measured under ambient conditions using an atomic force microscopy in ScanAsyst-Air mode and a silicon tip with a radius of 2 nm. Angle-resolved piezoresponse force microscopy imaging of the diagonal domains in the film was performed using a contact PtIr-coated silicon tip with a radius of 20 nm, a force constant of 2.8 N/m, and an alternating current signal at a frequency of 75 kHz and an amplitude of 10 V. Both the in-plane and out-of-plane domain images were captured after in-plane rotations of the sample at angles of 0° and 90°, respectively. Finally, a montage was used to convert all domains across the film area with the evolution of the applied voltages. The exposed wall currents at the film surface were investigated using contact mode conductive atomic force microscopy under a −5 V bias. Each current-voltage curve was measured using an Agilent B1500A semiconductor analyser operating in voltage sweep mode with a sweep time of 90 s.

Under an in-plane applied electric field over two top electrodes, partially switched domains within the gap, which enable the formation of conductive walls during the read operation, spontaneously retract when the read voltage is removed, reducing the accumulation of mobile defects at the domain walls and potentially improving the device stability. Three-terminal memory devices produced 14 nA read currents at an operating voltage of 5 V, and operated up to T = 85°C. Additionally, the $BiFeO_3$ (110)/$SrTiO_3$ (110) sample has a monodomain configuration, which provides a practical and feasible method to examine the correlation between the charge compensation and the local electrical conductivity of the domain walls. The wall current can be increased over 300 nA through the careful selection of current flowing paths along the charged walls, besides the enhancement of the conductive wall number through the local hierarchical evolution of the 71°, 109° and 180° domains. It is proved that 180° domain reversal proceeds by multiple 71° rotations of the pristine domains. This new concept device with the sufficient readout current is far less prone to the scaling issue raised for conventional charge-based ferroelectric memory and extended defect-based resistive memory.

Keywords: ferroelectric thin film; doman wall memory; multiple rotations

FA-43

反钙钛矿化合物 $Mn_3XN(C)$的“晶格-自旋”强关联及其负/零热膨胀行为研究

王聪[1]，孙莹[1]，王蕾[2]
1.北京航空航天大学
2.北京科技大学

反钙钛矿化合物 $Mn_3XN(C)$系列材料由于“晶格-自旋-电荷”的强关联性，发现诸多具有应用价值的物理特性，如零/负膨胀、压磁、磁热、磁致伸缩、巨磁阻、超导、近零电阻温度系数等。在 NMn_6 八面体中，Mn-Mn 直接交换作用和 Mn-X-Mn 间接磁交换作用共存，形成复杂的磁结构， 且其磁结构对成分、温度、压力、磁场等的变化非常敏感，因此在多场耦合下产生丰富的物理特性。我们利用中子衍射技术结合 Rietveld 精修原位测量并解析了这类化合物在不同外场下的晶体结构和磁结构,探讨“晶格-自旋”强关联的量化关系，此类化合物在化学掺杂、温度和压力场下的磁结构演变规律，以及诱导的物性变化，如铁磁-反铁磁转变、负（零）热膨胀、压磁、压热效应等。

关键词：反钙钛矿；中子衍射；负膨胀；零膨胀；压磁效应

FA-44

基于纳米结构的光电器件

范智勇
1.香港科技大学深圳研究院
2.香港科技大学电子与计算机工程系

由纳米/微米结构制成的材料具有独特的物理性质，例如快速载流子传输，高表面体积比，机械柔韧性，亚波长光波导等。这些有趣的特性可用于各种电子和光子学器件。我们制造了各种由纳米线，纳米柱，纳米锥等组成的阵列纳米结构，使用从无机半导体到有机金属钙钛矿材料的各种材料。这些纳米结构可以用纳米压印，化学气相沉积方法和打印方法来制造。我们对这些纳米结构的光学性质进行了系统的研究，揭示了光捕获的机理。同时，这些材料已被制造成各种光电子器件，包括光电探测器和太阳能电池。该研究表明，三维（3-D）阵列纳米结构可以帮助提高太阳能电池器件的能量转换效率以及柔性。同时研究表明，结构设计的优化具有相当的重要性。

关键词：纳米结构；太阳能电池；光电传感器

FA-45

Interplay of Ferroelectric Order and Itinerant Electrons in $LiOsO_3$

Feng Jin[1], Youguo Shi[2], Rong Yu[1], Qingming Zhang[2,3]

1.Department of Physics, Renmin University of China, Beijing 100872, China
2.Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
3.School of Physical Science and Technology, Lanzhou University, Lanzhou 730000, China

Ferroelectric distortion in a metallic state has long been thought experimentally inaccessible because itinerant electrons screen the long-range Coulomb interactions that favor a polar structure. However, the recent discovery of ferroelectric metal $LiOsO_3$ breaks the barrier imposed by the previous lack of real materials exhibiting the desired characteristics. In this system, the coexistence of ferroelectric order and itinerant electrons offers an unprecedented opportunity to explore exotic phenomena and establish new technological platforms. Here, we report the first experimental study of the interplay between ferroelectric order and itinerant electrons in $LiOsO_3$. Our comprehensive Raman experiments demonstrate that the ferroelectric ordering of the Li ions with decreasing temperature is significantly slowed by the itinerant electrons. On the other hand, transport measurements suggest that this ordering substantially enhances the anisotropy of charge transport. These observations are well explained by our effective pseudospin-fermion model that describes the interactions between the itinerant electrons and the ferroelectric dipoles. Furthermore, this model allows us to predict additional intriguing behaviors that may emerge in such a system. Our findings pave the way toward unveiling the fundamental physics of this ferroelectric metal and developing novel applications thereof.

FA-46

Spatial Distribution of the Degree of Crystallinity in Polymer films

Hanying Li
MOE Key Laboratory of Macromolecule Synthesis and Functionalization, State Key Laboratory of Silicon Materials, Department of Polymer Science and Engineering, Zhejiang University, Hangzhou, 310027, P. R. China.

The degree of crystallinity in polymer significantly affects the physical properties of polymer materials. However, the distribution of the degree of crystallinity in the polymer has never been considered even though it is equally important affecting the properties of polymer. Herein, we detect, for the first time, how the degree of crystallinity is distributed in polymer films utilizing the Raman spectrum. The results indicate that the degree of crystallinity is not uniform through the films but presents a distribution along the radial direction of spherulite. This work begins to provide an additional structural feature of crystalline polymers that should greatly affect the polymer properties and the associated applications.

FA-47

Strain Modulation to Ultrathin Ferroelectric Tunnel Junction Memory

Hei-Man Yau, Zheng Wen, Ji-Yan Dai
Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong

Strain engineering plays a critical role in ferroelectric memories. In this work, we demonstrate dynamic strain-modulation on tunneling electroresistance in ultrathin BaTiO3 or BST metal/ferroelectric/semiconductor tunnel junction by applying mechanical stress to the device. With an extra compressive strain induced by mechanical stress which is dynamically applied to the $BaTiO_3$ or BST layer and the Nb:$SrTiO_3$ substrate, the ON/OFF current ratio increases significantly, whereas a mechanical erasing effect can be observed when a tensile stress is applied. This dynamic strain engineering gives rise to an efficient modulation of ON/OFF ratio due to the variation of BaTiO3 polarization.

Acknowledgement This work was supported by the financial support of Hong Kong RGC (Grant: PolyU15309416) and PolyU Strategic Importance Project (Grant: 1-ZE25, 1-BBAF). Wen acknowledges the financial support of Natural Science Foundation of China (Grant No. 11574169) and the Hong Kong Scholars Program (Grant No. XJ2015024). Experiments were carried out in part in the University Research Facility in Materials Characterization and Device Fabrication, The Hong Kong Polytechnic University.

FA-48

Additive Manufacturing Porous Ti-6Al-4V Fusion Cage Investigations: Multi-scale Investigation for Biological Apatite Crystallites in Bone Remodeling and Mineralization

E-Wen Huang
National Chiao Tung University

Long term successful of spinal fusion cages made of metallic biomaterials is expected to effectively promote the mechanobiological process through the complete degree of bone incorporation as well as the rich osseointegration between the host bone and the implants. An optimal configuration of porous Ti-6Al-4V implant fabricated via the additive manufacturing of selective laser melting (SLM) was evaluated in complimentary structure examinations to investigate the growth of autologous osseous at multi-length scales. Microcomputed tomography (micro-CT) using newly-built analysis method indicates that the optimal design of porous Ti-6Al-4V fusion cage is much better for bone ingrowth at the microstructure level. The fluorescence and histological staining analyses as the standard protocols confirm the results obtained from micro-CT. We further employ complimentary small and wide angle X-ray scattering (SWAXS) to examine the bone mineralization and the crystallographic orientation distributions. Two characteristic structures of biological apatite at different length scales are investigated by synchrotron radiation x-ray at transition mode. The microscopy imaging modalities reveal that a much greater amount of new bone and mature bone is obviously achieved in the designed Ti-6Al-4V alloy compared to commercially non-porous titanium alloy and porous tantalum metal implants. All newly formed bone exhibits the isotropic orientation whereas mature bone obtained in Ti-6Al-4V reveals the preferential alignment of constituent apatite crystallites, indicating a fully mineralized mature bone around Ti-6Al-4V. In addition, higher crystallinity volumes are observed in the mature bone rather than the new bone. The high degree in bone remodeling and mineral crystallinity of the fully mature bone suggests a potentially promising alternative of additive manufactured Ti-6Al-4V implant in spinal fusion devices. The nondestructive synchrotron x-ray methods demonstrate the growth mechanisms.

Keywords: spinal fusion cage, implant, additive manufacturing, histology, fluorescence, microcomputed tomograp

FA-49

Femtosecond laser-colorized indium-tin-oxide films for blue light attenuation and image screening

Chih-Wei Luo
Department of Electrophysics, National Chiao Tung University

The need for ink- and toxin-free painting means that laser colorization using laser-induced periodic surface structures (LIPSSs) is important because it is environmentally friendly. Recently, LIPSSs have been observed on various materials and this type of surface structures also modifies some physical properties, such as the friction, the hydrophobicity/ hydrophilicity, the conductivity and the absorptance. Laser-colorized materials are realized by controlling the morphology. For example, a variety of colors for different metals (e.g., aluminum, stainless steel, etc.) and semiconductors (e.g., Ge) was demonstrated using a femtosecond laser processing technique. However, to the authors' best knowledge, there has been no attempt to colorize transparent conducting materials using femtosecond laser processing. This study shows that the color of indium-tin-oxide (ITO) films can be easily controlled using femtosecond laser processing. ITO is both transparent and conducting and is an important material for industrial applications in solar cells and touch panels. There have been many attempts to enhance the transparency and reduce the resistivity via femtosecond laser-induced crystallization. Precisely selective crystallization using laser annealing allows areas to be patterned and the line width of electrodes in touch panels to be reduced. Touch panels are indispensable devices for work, communication, and entertainment. Eye protection and the preservation of personal privacy is important issue for long-term usage.

This study fabricates various nanostructures on the surface of ITO films by using femtosecond laser processing to modify their optical properties. For high laser fluences (>646 mJ/cm^2), a densely cotton-like structure is formed on the surface and there is a cyan color. For laser fluences of ~200 mJ/cm^2, both cotton-like and nano-bricks are simultaneously formed on the surface and a yellow color is produced. When the laser fluences are less than 68 mJ/cm^2, only a nano-brick structure is formed on the surface and an orange color is produced. The changes in the reflectance and transmittance spectra for ITO films that are annealed using a femtosecond laser are strongly dependent on the surface morphology, which also results in a change in color. Previous studies have shown that femtosecond laser-induced nanostructures on ITO films enhance the conductivity, but also significantly modify the optical properties, as shown in this study. The significant reduction in transmittance in the blue-light region is good for eye protection. It is also demonstrated that laser-colorized ITO films with specific reflected light can block the image behind the laser-colorized ITO film, which has potential application for information panels, in terms of information security and the protection of privacy.

Keywords: ITO, laser-colorized, femtosecond laser processing, eye protection, information security

FA-50

Surface Coordination Chemistry of Metal Nanomaterials

Nanfeng Zheng
Collaborative Innovation Center of Chemistry for Energy Materials, State Key Laboratory for Physical Chemistry of Solid Surfaces, and Department of Chemistry, Xiamen University

The surface and interfacial structures of nanomaterials play crucial roles in determining their chemical properties. However, it remains challenging to characterize and precisely control the surface and interfacial structures of nanomaterials. In this presentation, I will discuss how the surface coordination chemistry controls the properties of metal nanomaterials at the molecular level (see the perspective in *J. Am. Chem. Soc*. 2017, *139*, 2122). The mechanism on how small ligands help to control the surface structure and thus catalysis of metal nanocrystals will be discussed. Some examples will also be given toward understanding the significant steric and electronic effects of surface ligands on promoting the catalysis of metal nanomaterials, particularly their catalytic selectivity (*Chem* 2018, *4*, 1080; *Nature Mater.* 2016, *15*, 564). Finally, two synthetic strategies to create model catalysts for resolving the detailed metal-support interfacial structures will be presented (*Science* 2014, *344*, 495; *Science* 2016, *352*, 797)

FA-51

Functional Mesoporous Materials Templated by Block Copolymers

Shiao-Wei Kuo
National Sun Yat Sen University

Recently, we have utilized several unique amphiphilic block copolymers as templates, such as PE-PEO, PEO-PCL, PE-PEO-PCL, and PEO-PCL-PLLA to successfully fabricate a series of mesoporous materials, for example, mesoporous silicas, mesoporous phenolic resins and mesoporous carbons by a convenient EISA method. Firstly, we took PE-PEO as model block copolymer to study the TEOS-to-template or HCl-to-template weight ratio effect during the EISA process, view from the thermal dynamic point and kinetic reason, respectively. In addition, we expended the research method to the other block copolymer systems, especially for the unusual ABC type triblock copolymers, we obtained the hierarchical mesostructure by single template. These specific mesostructures could be observed easily by small angle X-ray scattering (SAXS), transmission electron microscopy (TEM) and isotherm N2 experiment. Moreover, blending technique could also be used in the templating process during EISA, the clear method could easily control the morphology and pore size of the mesoporous materials.

Keywords: Hydrogen Bonding, Block Copolymer, Mesoporous Materials, Self-Assembly

FA-52

Doped Semiconductor Nanocrystals and Their Hetero-structures

Jiatao Zhang
1.Beijing Institute of Technology
2.Beijing Key Laboratory of Construction Tailorable Advanced Functional Materials and Green Applications

The precise control of doping and hetero-interface induced band gap engineering, in colloidal semiconductor nanocrystals (NCs), is very important for the efficient energy or charge transfer through hetero-interface and then their novel optoelectronic properties exploration and their new energy, new optoelectronic devices applications. Deep-position aliovalent doping in NCs and the growth of monocrystalline semiconductor based metal/semiconductor hybrid nanocrystals (core/shell and heterodimer) with modulated composition, morphology and interface strain are the prerequisite for controlling of electronic impurities, the plasmon-exciton coupling, efficient electron/hole separation, and enhanced new energy conversion applications. We realized the aliovalent doping and nanoscale monocrystalline growth of the semiconductor shell on metal nanocrystals, the precise substitutional dopant and hetero-interface to metal nano-building-blocks have been realized in our group by novel cation exchange strategy. These controls enable the fine tuning of doped level, plasmon-exciton coupling, Plasmon enhanced photocatalytic performance and enhanced photovoltaic, electrical properties applications.

Keywords: colloidal nanocrystals; quantum dots, doping; hetero-structures, heterointerface

FA-53

Free-standing Planar Thermoelectric Microrefrigerators based on Nano-grained SiGe Thin Films

Yu Su, Baoling Huang

Department of Mechanical and Aerospace Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

Rapid development of modern miniaturized microelectronic and optical devices demands for low-power and fast-response on-chip refrigeration to reduce thermal noise and improve device lifetime. Thermoelectric microrefrigerators offer an attractive all-solid-state solution with many prominent merits. Conventional thermoelectric microrefrigerators widely adopt integrated-circuit (IC)-incompatible toxic heavy metal compounds as thermoelectric elements, rendering them unsuitable for on-chip integration. Here we developed free-standing planar thermoelectric microrefrigerators based on nanograined SiGe thin films. The novel support-free design and the record high performance of the nanograined SiGe thin films lead to significant improvement in the cooling performance. A maximum cooling temperature of 10.3 K together with a response time of 16 ms has been achieved in the single-stage microrefrigerator with a power consumption of 56 μW near room temperature while a maximum cooling temperature of 11.2 K can be achieved in the two-stage refrigerator with 0.41 mW input power. The cooling temperatures of the SiGe microrefrigerators also improve with the increasing ambient temperature, reaching up to 15 K and 17 K for the single and two-stage microrefrigerators respectively at 340 K. These SiGe thin-film devices can deliver cooling performances comparable to the records for traditional heavy-metal-based microrefrigerators while providing excellent IC compatibility and almost one to two orders of magnitude higher cooling temperature to power consumption ratios (184 K/mW), rendering them ideal candidates for low-power on-chip refrigeration.

FA-54

金属-有机框架催化材料的构筑和性能

曹荣

中国科学院福建物质结构研究所

FA-55

Polymer-Assisted Metal Deposition for Soft Electronics

Zijian Zheng

The Hong Kong Polytechnic University

Metal electrodes are indispensable element for most future soft electronic devices. One critical challenge in this field is how to fabricate highly conductive, adhesive, smooth, and soft metal conductors at low temperature under ambient conditions, and preferably in a roll-to-roll manner. Our laboratory recently develops Polymer-Assisted Metal Deposition (PAMD) to address this issue. PAMD allows ambient fabrication of flexible, foldable, stretchable, compressible, and wearable metal (especially Cu) conductors with very high conductivity. Importantly, PAMD is compatible with versatile substrates and different printing technologies at ambient conditions. This seminar will discuss the materials chemistry of PAMD and demonstrate their applications in several important soft electronic devices including circuits, solar cells, supercapacitors, and transistors.

FA-56

上转换纳米晶中浓度猝灭问题的研究

王锋

香港城市大学深圳研究院

稀土掺杂上转换纳米晶因具有一系列独特的光谱性质而在照明、显示、激光、光伏、以及生物医学等方向产生了巨大的影响。这类材料不仅能够替代传统荧光染料和半导体量子点进行高灵敏的生物监测和高质量的生物成像，还能实现基于活体的光学图像构建和光控释药。然而实际应用大多受制于上转换纳米晶的低发光亮度，源于纳米晶的低掺杂浓度。本报告将介绍我们课题组通过核壳结构设计遏制高掺杂浓度下的浓度猝灭，从而提高上转换的发光亮度，并进而拓展其在前沿技术中的应用。

关键词：上转换；浓度猝灭；核壳纳米结构

FA-57

Morphology of Fused Ring Electron Accepters and Their Applications

Xinhui Lu
The Chinese University of Hong Kong

Non-fullerene acceptors, which are emerging as replacements for conventional fullerene derivatives, offer complementary absorption spectra to those of donor materials, adjustable energy levels, and batch-to-batch reproducibility. In this work, we are going to present our recent work on the bulk morphology of several fused ring electron acceptors investigated by grazing incidence X-ray scattering techniques. Furthermore, we employed ITIC-Th, which belongs to this family, to stabilize the perovskite precursor solution containing mixed cations and halides. We find that ITIC-Th can effectively suppress the formation of photo-inactive yellow non-perovskite phase (δ-phase) in the films made from the aged precursor solution. As a result, the devices fabricated from the aged precursor solution with ITIC-Th experience much less efficiency drop with the increase of the aging time of the precursor solution.
Keywords: non-fullerene electron acceptor, morphology, GIWAXS, organic solar cell, perovskite solar cell

FA-58

The application of material analysis on IC industry

榮欽 Chen, Chao-Wei Chen, Yu-Han Chen, Cheng-Hsing Chen, Cheng-Huang Yang, Bang-Hao Haung, Shih-Hsin Chang
MSSCORPS CO., LTD.

For research and development (R&D), material analysis plays a crucial role not only in academia but in industry. It becomes more and more important and challenging especially for integrated circuit (IC) because of continuously scaling of fabrication dimension down to few nanometers. For such aggressive technology node, material analysis tools with high-spatial resolution are needed. In this presentation, two high-end material analysis tools, transmission electron microscopy (TEM) and energy dispersive X-ray spectroscopy (EDS), are introduced to analysis two mobile phone CUPs, A11 Bionic (iPhone 8) and Exynos8895 (Samsung S8). The technology node for these two chips is 10 nm FinFET, fabricated by tsmc and Samsung, respectively. With the help of TEM and EDS, subtle differences about Fin structure and dimension as well as chemical information can be clearly identified and analyzed. More applications of material analysis will be presented and discussed during the presentation.
Keywords: TEM

FA-59

The Application of 2-D materials in organic or hybrid solar cells

Feng Yan
The Hong Kong Polytechnic University, Department of Applied Physics

Graphene has shown promising applications in photovoltaic devices for its high carrier mobility and conductivity, high transparency, excellent mechanical flexibility and ultrathin thickness, and has been used in solar cells as transparent electrodes or interfacial layers. Other 2-dimensional (2-D) materials also show some fascinating physical properties due to the 2-dimensional nature. In this talk, I will introduce our recent work on the applications of graphene and other 2-D material in organic or perovskite solar cells as follows. (1) Semitransparent perovskite solar cells are prepared by laminating graphene transparent electrodes on the top for the first time. The device performance is optimized by improving the conductivity of the graphene electrodes and the contact between the graphene and the perovskite active layers during the lamination process. The devices show high power conversion efficiencies when they are illuminated from both sides. (2) Solution-exfoliated few layers black phosphorus (BP) and MoS_2 flakes are served as effective charge transport layers in perovskite solar cells, which can improve the device performance due to the passivation of grain boundaries of perovskite active layers and the enhancement of charge transfer. (3) Ultrathin flexible perovskite solar cells were prepared by introducing graphene transparent electrodes. The devices show excellent bending stability and high power output per weight. All of the works demonstrate promising applications of 2-D materials in perovskite solar cells and pave a way for improving perovskite solar cells as well as other types of photovoltaic devices by utilizing novel 2-D materials.

FA-60

晶圆级单层硫化钨及其在高性能柔性光电探测器中的应用

何頌賢
City University of Hong Kong

近年来，由于在新型电子器件和光电子器件等方面中具有光明的应用前景，二维材料引起了研究人员的极大关注。然而，二维材料的大规模应用却依赖于其大面积合成。本研究发现，采用多温区管式炉，前驱体的蒸气压可以得到有效调控，进而可以通过增强化学气相沉积法获得具有晶圆尺度（两英寸）的均匀单层硫化钨薄膜。基于该薄膜的光电探测器具有优良的性能，其光响应度为 0.52 mA/W，探测度高达 4.9×10^9 Jones，且响应速度快，小于 560 μs。当将薄膜转移到聚酰亚胺柔性衬底上构成柔性光电探测器后，其光响应度增强一个数量级，高达 5 mA/W。更为重要的是，当弯折 3000 次后，其光电流可以保持为最初状态的 89%。以上结果表明本合成方法不仅可以拓展到合成更大面积的均匀单层硫化钨，而且所合成的硫化物具有优良的机械柔性，使其在柔性光电子器件方面具有广阔的应用前景。

关键词：晶圆级；硫化钨；柔性；光电探测器

FA-61

原子层沉积技术制备新型纳米薄膜材料

王新炜

北京大学深圳研究生院

原子层沉积（ALD）技术是一种气相薄膜沉积技术，它利用饱和自限性的表面化学反应，使薄膜材料在原子层尺度上逐层可控生长。ALD 所得的薄膜在大面积尺度上具有高度的均匀性，并可在复杂多孔的三维结构上实现高度保形的薄膜包覆。这些独特的优势使得 ALD 技术近些年来应用在越来越多的纳米材料设计和制备中。但是，目前 ALD 技术所能实现的材料种类还有一定的局限性，尤其在铁钴镍硫化物方面，相关的研究还较非常初步。

在本报告中，作者将主要介绍近几年来我们在 ALD 新材料与新工艺研究方面的成果。我们开发了硫化铁、硫化钴、硫化镍等一系列新型硫化物材料的 ALD 工艺，并将其应用在超级电容器、电催化水制氢制氧等多种能源存储与转化器件中。我们也开发了氧化钒、金属铜等材料的低温 ALD 工艺，可以在 50 摄氏度实现高质量 ALD 薄膜的制备。我们进一步将低温 ALD 工艺应用于有机薄膜晶体管器件中，可显著降低有机层与金属电极之间的接触电阻。

FA-62

导电聚合物/碳纳米管或石墨烯复合热电材料

陈光明

中国科学院化学研究所

我们首次采用“单体吸附-原位聚合”法制备了 PEDOT/石墨烯复合热电材料，并进而发展了三种化学氧化聚合过程；采用原位聚合法制备了 PEDOT/CNT、PPy/CNT 和 PPy/石墨烯复合材料，详细研究了 PEDOT 或 PPy 在石墨烯或 CNT 表面的包覆形貌与界面相互作用；可控构筑了 PEDOT 微纳米球、棒、管和纤维以及 PPy 微纳米结构，发现材料的热电性能对其微纳米结构具有强烈的依赖性，并研究了硫酸等后处理对微纳米结构热电性能的影响；构筑了 PPy 纳米线/石墨烯三维网络结构，得到了具有层状形貌的 PPy 纳米线/CNT 复合材料，以及具有珊瑚状形貌的 PEDOT/SWCNT 复合材料，这些复合材料具有优异的热电性能；无需合成特定单体，制备了热电性能高度可调的新型席夫碱聚合物/CNT 复合热电材料；采用系列有机小分子，对 SWCNT 进行有机化处理，得到高性能 n-型或 p-型复合热电材料；制备了石墨烯/SWCNT 复合热电气凝胶和热电化学聚合物复合水凝胶热电材料；基于该部分工作，申请人应主编邀请，对近年来的研究结果进行总结，并发表了 2 篇综述。

致谢：国家自然科学基金（No.：51573190）资助。

关键词：热电材料；导电聚合物；碳纳米管；石墨烯；复合材料

FA-63

Optical properties of chiral plasmonic nanoparticles

Junjun Liu, Ling Yang, Zhifeng Huang

Hong Kong Baptist Unviersity

The generation of helical metamaterials, which have strong, engineerable chiroptical activity in the UV–visible region, has attracted increasing attention due to the manipulation of the circular polarization state of light to develop diverse homochirality-associated bio-applications. Glancing-angle deposition with fast substrate rotation is performed to generate plasmonic helical NPs (PhNPs) with a helical pitch (P) of less than 10 nm, which is so much smaller than the wire diameter (d) that the PhNPs appear to be achiral NPs. The PhNPs exhibit chiroptical activity that originates intrinsically from hidden helicity, characterized by circular dichroism (CD). With an increase of P from 3 to 66 nm, the plasmonic CD signals barely shift but show a logarithmic

amplification. PhNPs made of aluminum, silver, and copper exhibit a stable chiroptical response from the deep UV (~220 nm) region to the visible region. When an achiral plasmonic nanostructure guest is coated on a PhNP host (i.e., a chiral host@achiral guest nanostructure is created), the achiral guest becomes chiroptically active due to helicity transfer from the chiral host to the achiral guest. Such a helicity transfer can be generally adapted to diverse plasmonic metals to tailor the plasmonic chiroptical response flexibly in the UV–visible region. Furthermore, an amplification of the near-field optical chirality induced by the PhNPs would pave a novel way to performing asymmetric syntheses, for which investigations are currently lacking. Silver PhNPs are used to effectively mediate the enantioselective photocyclodimerization of 2-anthracenecarboxylate: left-handed silver PhNPs lead to a positive ee (enantiomeric excess) value, and right-handed silver PhNPs give rise to a negative ee value. The enantioselectivity is enhanced with a decreasing P. The PhNP-mediated enantioselective photocyclodimerization is ascribed to the synergistic contribution from chirally helical surface-induced enantioselective adsorption of 2-anthracenecarboxylate and chiroptically active nanoplasmon-enhanced optical chirality of near-field circularly polarized light.
Keywords: chiral plasmonics, hidden chirality, GLAD

FA-64

Phase selection during solidification of colloidal suspensions

Jiaxue You[1], Jincheng Wang[1], Zhijun Wang[1], M. Grae Worster[2]
1.State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi’an 710072, P. R. China
2.Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Colloidal particles are forced into a variety of morphologies when a suspension is frozen: soil is compacted between ice lenses during frost heave; ice templating is a growing technology to produce bio-inspired, micro-porous materials; cells and tissue can be damaged during cryo-surgery; and new energy materials and various advanced composites with tailored microstructure can be fabricated by freeze casting. However, the dynamics of pattern formation in solidification of colloidal suspensions remain poorly understood. Here, we develop a theoretical model to predict the phase selection of frozen fringes, laddered structures and dendrites. A series of experiments are performed to confirm the model. We find that the structures of this complex freezing system are determined by the interplay of forces and thermodynamics of the particulate system. An instructive phase diagram is given to identify experimental parameters that differentiates between these structures, and unify a range of apparently disparate conclusions drawn from previous experimental studies.
Keywords: colloidal suspensions, solidification, phase selection, theory and experiments

FA-65

New Rare‐Earth Metal Germanides with Two-dimensional Germanium Network Modulation Structure

Jiliang Zhang[1,3], Guangcun Shan[2,3]
1.City University of Hong Kong, Hong Kong SAR & Dongguk University, South Korea
2.Beihang University
3.City University of Hong Kong, Hong Kong SAR

Rare-earth Germanides have complex structural and chemical properties and therefore exhibit many interesting physical properties such as magnetism, superconductivity, and heavy Fermion. In this work, the modulation structures and properties in a series of rare earth germanides induced by vacancies and microalloying were investigated by using single-crystal X-ray diffraction and electron diffraction as main methods. The Ge-vacancy does not produce the expected disordered structure, which instead produces a series of long-range ordered modulation structures with the two-dimensional network. Aluminum micro-alloying does not produce rare-earth di-germanides and tri-germanides with interstitial solid solution, which leads to the deformation of the two-dimensional network and the formation of one-dimensional structure, thereby inducing new modulation structures. Electron diffraction results show that, depending on the rare earth elements, the modulation structure can be either Incommensurate or non-Incommensurate. The analysis of the crystal structures and the electronic structures shows that the generation of the modulation structures is related to the sp2 hybridization and the Peierls distortion.
Keywords: Rare-earth Germanides, two-dimensional Germanium network, modulation structure

FA-P01

Evolution of Local Strain at MoS_2-Metal Boundaries: the Effect of Substrate Interaction

Moe Yan Aung, Yinghui Sun, Rongming Wang
University of Science and Technology Beijing

Atomically thin two-dimensional (2D) materials attract intensive attention for their applications in nano-electronics. The study on stress-strain related properties is of vital importance for material optimization. Strain is an unavoidable factor in delicate device fabrication and can also be utilized to tune the device performance. The deposition of metal nanoparticles can induce both local strain at the metal-MoS_2 boundary and surface plasmon resonance effect. The induced strain can further affect the electronic and optical properties of 2D materials and the devices.

The evolution of local strain induced by the Ag nanostructure on different layers of MoS_2 are investigated in this work. The trend of the strain relaxation is helpful for understanding both the inter-layer interaction and the substrate interaction. Scanning electron microscopy and X-ray photon spectroscopy were employed to characterize the electrical and morphological changes of the interfaces. The intensity and position changes of Raman peaks influenced by the local strain show that the strain lasts longer in monolayer MoS_2, compared with that in the few layer MoS_2. The speed of strain relaxation is monotonically increased with the layer number of MoS_2. Our results provide detailed studies on the surface interactions including MoS_2-MoS_2 interface and MoS_2-substrate interface, and may contribute to the optimal application of MoS_2 in future device fabrications.

Keywords: MoS_2, metal induced strain, strain relaxation, substrate ineraction, Raman spectroscopy

FA-P02

Microstructure, Optical, and Scintillation Properties of Ce:$Gd_2YAl_2Ga_3O_{12}$ Transparent Ceramics

Shuilin Chen[1,2], Benxue Jiang[1], Long Zhang[1]
1.Key Laboratory of Materials for High Power Laser, Shanghai Institute of Optics and Fine Mechanics, CAS, Shanghai 201800
2.University of Chinese Academy of Sciences, Beijing 100049, China

Inorganic scintillator materials are widely use in neutron detect, high energy particle physical experiments, new energy resource exploration and X-ray security, especially in medical imaging techniques (computed tomography and positron emission tomography). In this study, Cerium doped $Gd_2YGa_3Al_2O_{12}$ (GYGAG) ceramic with good performances have been fabricated by sintering in oxygen atmosphere and hot isostatically pressed (HIP). The microstructure, optical, scintillation characteristics of Ce:GYGAG ceramic were investigated. Transparent ceramic Ce:GYGAG ceramic achieves 78% transmittance in range from 500 to 800 nm. The photoluminescence emission of the Ce:GYGAG ceramic peaked at about 540 nm match well with the sensitivity of Si-based photodiodes. Radio-luminescence intensity of the fast emission based on Ce3+5d→4f reaches up to 30 times that of BGO single crystal reference scintillator. The light yield within 0.75μs shaping time in Ce:GYGAG ceramic is about 23400Ph/MeV under the 137Cs γ-ray irradiation. The result of using electron paramagnetic resonance indicate that there are Ce^{4+} ions in the oxygen-annealed Ce:GYGAG scintillator ceramics. The valence of Ce ions in the oxygen-annealed and hydrogen-annealed Ce:GYGAG scintillator ceramics was confirmed by X-ray photoelectron spectroscopy. Finally, the scintillator performance affected by the different of anneal atmospheres are discussed.

Keywords: Ce:GYGAG, scintillator ceramic, anneal atmosphere

FA-P03

Stability Investigation of Pt_1/α-Fe_2O_3 Single-atom Catalyst with High Number Density Under Gas Environments

Sibin Duan[1], Jingyue Liu[2], Rongming Wang[1]
1.Beijing Key Laboratory for Magneto-Photoelectrical Composite and Interface Science, School of Mathematics and Physics, University of Science and Technology Beijing, Beijing 100083, China
2.Department of Physics, Arizona State University, Tempe, Arizona 85287, United States

Single atom catalysts (SACs), which maximize the efficiency of precious metal compounds, play an important role in both fundamental research and industrial applications. Because of the high surface free energy, high loading levels of isolated single metal atoms are not stable and easy to sinter into larger particles or small clusters during practical catalytic reactions. Research into the stability of supported single atom during catalytic reaction will benefit the understanding of the sintering mechanism and promote the development of stable SACs to boost their industrial application. Here, the high number-density Pt SACs were synthesized by a modified adsorption method. Aberration-corrected high-angle annular dark-field microscopy under scanning model (HAADF-STEM) was used to characterize the fresh and used catalysts. The atomic resolution HAADF-STEM images reveal only isolated Pt single atoms uniformly dispersed onto the surfaces of α-Fe_2O_3 nanocrystallites in the fresh sample. Investigation on the stability of Pt atoms under different gas environments suggests that the Pt atoms are stable under an oxidative atmosphere. Reductive gas including H_2 and CO weakens the metal–support interaction and induces the movement of Pt atoms, forming nanoparticles or clusters. The weakening effect of H_2 is proven to be stronger than that of CO and will be further enhanced by the addition of water into the feed gas. These findings will benefit the research on the stability of SACs during catalytic reactions and instruct the design of SACs with more stable anchoring sites.

Acknowledgments: This research was supported by the National Natural Science Foundation of China under 11280121, the Beijing Municipal Science and Technology Project (No. Z171110000221707 4), and the Fundamental Research Funds for the Central Universities under FRF-TP-16-067A1.
Keywords: single-atom catalyst, stability, metal-support interaction

FA-P04

Effects of Sample-size on the Compression Deformation Behavior of a CuZr-based Bulk Metallic Glass Composite

Yongsheng Chen, Weizhong Liang, Longxing Wang, Xinchi Liu
Heilongjiang University of Science and Technology

Compressive deformation behavior of $Cu_{45}Zr_{48}Al4Nb_3$ bulk metallic glass composite with different diameters was systematically investigated. It was found that smaller sample not only exhibited a larger yield strength but also had a higher compressive plasticity. With the increase in sample size, cooling rate and the glass transition temperature reduced. The yield strength was found to depend on the volume fraction of crystalline phases in the glassy matrix. The smaller sample had a larger amount of free volume, which was found to favor plastic deformation. The results showed that the deformation behavior was sensitive to sample size. The results may be helpful for the investigation of metallic glass composite mechanical behavior.

Keywords: Bulk metallic glass composite; Sample size; Deformation behavior; Plasticity

FA-P05

Advanced Lithium Metal Anodes Based on 3D Hierarchically Porous Metals

Yifeng Cheng, Xi Ke, Zhicong Shi
Guangdong University of Technology

Rechargeable lithium metal anodes (LMAs) are key materials for the next generation high-energy-density secondary batteries. However, uncontrollable growth of Li dendrites leads to a low coulombic efficiency and poor safety. Herein, we develop a strategy for constructing a highly porous metal architecture on porous substrates, such as copper foam, as 3D hierarchically porous current collectors for LMAs. These current collectors exhibit significantly improved Li plating/stripping behavior owing to their uniform surface and capability of accommodating Li in the 3D HPC structures, which effectively suppresses the growth of Li dendrites. The Li@Cu/$LiFePO_4$ cell exhibits a high reversible capacity of 115 mAh g-1 with a high coulombic efficiency of 99.7% at 2 C for 500 cycles. The enhancement of the electrochemical performance of the LMAs based on 3D HPC/CF demonstrates the effectiveness of the design principles of 3D hierarchically porous current collectors for developing advanced LMAs.

FA-P06

Dispersion Study of Aramid Pulps in Epoxy Resin System

Xiaoma Ding, Haijuan Kong, Mengmeng Qiao, Zhifeng Hu, Muhuo Yu
Donghua University, Songjiang District, Shanghai

In order to improve the dispersion of a certain type of aramid pulps in epoxy resin system, the surface cleaning, dimension control, freeze-drying and product opening of the aramid pulps were processed in this experiment; In addition, the aramid pulp

reinforced epoxy resin composites were prepared by mixing the untreated and treated aramid pulps with epoxy resin system. The aramid pulps and their dispersion behavior in the epoxy resin system were characterized by scanning electron microscope (SEM), fiber quality analyzer (FQA), specific surface area tester (SSAA) and optical microscope (OM), at the same time, the tensile strength, fracture toughness, surface and typical fracture section of composites were tested and characterized by electronic universal material testing machine and scanning electron microscope (SEM). The results showed that, compared with untreated aramid pulps, the length distribution of the treated aramid pulps was more concentrated, the surface area was increased by 199%, the surface fibrillation degree has been greatly improved and its dispersion in epoxy resin system was more uniform; In addition, compared with the pure resin system (65.45MPa), when the aramid pulp content was 0.5wt%, the tensile strength of the untreated and treated aramid pulps reinforced epoxy resin composites were reached to a maximum of 76.12MPa and 79.36MPa, which were increased by 16.30% and 21.25% respectively; Similarly, compared with the pure resin system (0.86 MPa·$m^{1/2}$), when the aramid pulp content was 0.7wt%, the fracture toughness of the untreated and treated aramid pulps reinforced epoxy resin composites were reached to a maximum of 1.45MPa·$m^{1/2}$ and 1.68 MPa·$m^{1/2}$, which were increased by 68.60% and 95.35% respectively. Finally, through the SEM observation of the composite surface and typical fracture section, we found that the dispersion of the treated aramid pulp in epoxy resin system was more uniform and it was more reliable with epoxy resin system.

Keywords: Aramid pulp, Epoxy resin system, Dispersion, Tensile strength, Fracture toughness.

FA-P07

Room Temperature Tensile Deformation Behavior of a Ni-based Superalloy with High W Content

Guichen Hou, Jun Xie, Shuling Xun, Fengjiang Zhang, Zhenjiang Wang, Minghui Tan, Jinjiang Yu, Xiaofeng Sun, Yizhou Zhou
Institute of Metal Research, Chinese Academy of Sciences

Because of possessing good oxidation resistance, heat-resistant capability and good mechanical properties, the Ni-based superalloys with high W content have been widely used for preparing gas turbine vanes and high temperature forging dies. In this study, about 16 % (mass fraction) W contain in the Ni-base superalloy. The tension tests of the alloy are carried out at room temperature, and the microstructure of the fracture alloy are observed by means of optical microscope (OM), scanning electron microscope (SEM) and transmission electron microscope (TEM), so as to investigate the tensile deformation behavior of the Ni-based superalloy. The results show that the microstructure of the alloy consists of γ matrix, γ′ phase, eutectic, MC and M_6C carbides. The average yield strength and tensile strength of the alloy are 749 MPa and 975 MPa, respectively. And the corresponding elongation and reduction of area in the fracture alloy are measured to be 6 % and 9 %, respectively. During room temperature stretch, the deformed dislocations are activated in the matrix, and the moving dislocation can bypass γ′ phase by Orowan mechanism or shear into γ′ phase. Thereinto, the <110> super-dislocations shearing into γ′ phase can form the anti-phase boundary coupled two (1/2)<110> partial-dislocations (the corresponding reaction as follow <110>→(1/2)<110>+APB+(1/2)<110>) or decompose into the configuration of two (1/3)<112> partial dislocations plus stacking fault (namely, <110>→(1/3)<112>+(SF)+(1/3)<112>). In the later stage of tensile test, the slip-lines with different orientation are activated in the grain to promote the stress concentration in the regions of block carbide or the porosity, and the crack can initiate and propagate along these regions.

Keywords: Ni-based superalloy with high W content; microstructure; tensile behavior; deformation feature

FA-P08

Study on the Joints Properties of Aluminum Foams/Aluminum Plate by Transient Liquid Phase Bonding Process

Bensheng Huang, Xiong Wen, Xing Zhao, Guangwen Li
College of Materials Science and Engineering, Southwest Petroleum University

Aluminum foams/aluminum plate was transient liquid phase diffusion bonded with Cu/Al/Cu composite interlayer, then the investigation on joint microstructure, element diffusion and joint strength was conducted at 565℃. The results showed that, there was a significant grain boundary penetration phenomenon near the interface and it was more seriously at the side of aluminum foams. The XRD results showed indicated that the main phases near the interface were α-Al, $CuAl_2$, AlCu, Al_4Cu_9, Al_2O_3. By EDS line scanning, it indicated that the diffusion behavior of elements was different at three regions, compared with the edge region, the interface of the central region was better and the depth of element diffusion is larger, at the pore region, the liquefaction of interlayer was not successfully and the morphology was lamellar. Mechanical properties test showed that the largest shear strength of joint was 4.61

MPa when the duration was 40 min.

Keywords: Aluminum foams; transient liquid phase bonding; microstructure; element diffusion; shear strength

FA-P09

Investigation of the {10-12} twin in the Mg-Gd-Zn alloy

Yu Liu[1,2], Nana Wang[1,2], Hongtao Liu[1,2], Tao Lin[1,2], Jixue Zhou[1,2]

1.Advanced Materials Institute, Qilu University of Technology (Shandong Academy of Sciences)

2.Qilu University of Technology (Shandong Academy of Sciences), Shandong Provincial Key Laboratory for High Strength Lightweight Metallic Materials

The microstructure of the solid solution treated Mg-Gd-Zn alloy was investigated. After solid solution at 773K for 16 hours, a large amount of long period stacking ordered structures precipitated. The evolution of the microstructure indicated that the alloy had great solid solution strengthening effect. Besides, particles rich in Gd and Mg element were dispersed in the specimen. Both the long period structures and the particles were analyzed by the selected area electron diffraction technique. The annealing twins were observed in the specimen aged at 623K for 0.5 hour and the interface between the twin variant and the a-Mg matrix was studied. The stacking faults in the twin variant were investigated and the result showed the stacking faults were vertical to the (0002)a of the magnesium matrix.

Keywords: Mg-Gd-Zn alloy; solid solution strengthening; LPSO structure; annealing twins; interface

FA-P10

Au/NiS$_x$ Heterostructures: Controlled Growth and Structure-dependent Catalytic Performances for Hydrogen Evolution Reaction

Yuepeng Lv, Sibin Duan, Rongming Wang

Beijing Key Laboratory for Magneto-Photoelectrical Composite and Interface Science, School of Mathematics and Physics, University of Science and Technology Beijing, Beijing 100083, China

Nickel sulfides as promising catalysts towards hydrogen evolution reaction (HER) have attracted much interest.However, the reported HER catalytic activities of NiSx are relative low for their poor electrical conductivity. Constructing heterostructures consisting of noble metal and semiconductor has been proven to be an efficient method to promote their physicochemical performances benefitting from synergistic effects in the metal-semiconductor interface. Here, it was reported a controlled synthesis of Au/NiSx heterostructures with different architectures, i.e., core@shell, yolk/shell, and oligomer-like nanostructures in a one-pot synthesis procedure. The core@shell Au@NiS$_x$ nanoparticles are synthesized by seeded growth methods, while the yolk/shell Au/NiSx nanoparticles are prepared by in-situ transformation from Au-Ni bimetallic heterodimers. The Kirkendall effect determines the formation of yolk/shell structure with an empty space around the Au core rather than the core@shell structure. The structure-dependent HER catalytic performances of Au-modified NiS$_x$ nanoparticles were further investigated. The synergistic effect of the metal-semiconductor interface is confirmed to be superior to their oligomer-like counterpart. The overpotential of Au/NiS$_x$ nanoparticles with core@shell and yolk/shell nanostructures reach 253 mV and 263 mV at 10 mA/cm2 respectively, which are lower than those of oligomer-like Au-NiS$_x$ (283 mV) and NiS$_x$ (321 mV). These findings provide a new way to improve HER catalytic performances by elegant design of novel nanostructures.

Acknowledgements: This research was supported by the National Natural Science Foundation of China under 11280121, the Beijing Municipal Science and Technology Project (No. Z1711100002217074), and the Fundamental Research Funds for the Central Universities under FRF-TP-16-067A1.

Keywords: nickel sulfide, metal-semiconductor structure, HER, structure-property relationship

FA-P11

Effect of FSP on the Microstructure and Mechanical Property of Al-Mg Alloy

Yongqiang Qin[1,2], Congcong Meng[1], Feifei Liu[1], Shiang Zhou[1,2], Jun Huang[1,2], Yucheng Wu[1,2]

1.Hefei University of Technology

2.Laboratory of Nonferrous Metal Materials and Processing Engineering of Anhui Province

Al-Mg alloys have been widely used in the field of food handling and chemical processing industries because of their attractive

comprehensive properties such as medium strength, high ductility and excellent corrosion resistance. The strength of these alloys is primarily due to solid solution strengthening by Mg, which has a substantial solid solubility in aluminum. The main purpose of this study is to modify the surface structure of as-cast Al-5Mg alloy by friction stir processing (FSP) , and investigate its effect on the micro-structural and mechanical properties in detail. Particular emphasis was placed on the use of electron backscatter diffraction (EBSD) in order to further reveal the structural evolution of the alloy after FSP and the corresponding grain distribution in the studied alloy.

In our present work, a fine-grain microstructure was clearly observed in the Al-5Mg alloy due to the FSP. Scanning electron microscopy (SEM), electron back-scatter diffraction (EBSD) and properties testing were employed to investigate the structural evolution of these different regions and their effect on mechanical properties of the alloy. The following conclusions can be drawn: The as-cast Al-5Mg alloy exhibits a typical dendritic microstructure inside the coarse grains. Due to the high temperature generated by intense stirring effect, the FSPed alloy shows a complex macrostructure consisted of the base metal (BM), the heat-affected zone (HAZ), thermo-mechanically affected zone (TMAZ) and the nugget zone (NZ).The microstructure of the NZ region is characterized by fine equiaxed grains structure with a much smaller grain size of about 11.8μm, resulting in the simultaneously increase of the strength and ductility of the alloy.FSP improves an attractive comprehensive property of as-cast Al–Mg alloy. The tensile strength, yield strength and elongation of the FSPed Al-5Mg alloy are 344.7 MPa, 200.8 MPa and 35%, respectively.

Keywords: Al-Mg alloy; Friction stir processing; Microstructural; Mechanical properties

FA-P12

Basic Issues for High Pure Titanium Extraction Through Molten Salt Electrolysis

Jianxun Song, Shu Yongchun, He Jilin

Henan Province Industrial Technology Research Institute of Resources and Materials

High pure titanium which is a critical material used for integrated circuit (IC) manufacturing can be extracted by molten salt electrolysis process. It will be widely used in the future for the process is simple and easy to achieve continuous production. However, some scientific questions need to be clarified at present. 1. Current efficiency needs to be enhanced by way of electrolyte designing and selection; 2. Product quality needs to be improved by means of electrolyte purification; 3. Electrolytic parameters need to be optimized for obtaining a better morphology. Above on, this paper aims to explore the behaviors of titanium ions in various molten salts by means of chemical analysis, High-temperature Raman analysis and electrochemical testing. In the paper, concentrations of titanium ions were investigated and the molar ratios of complexes were analyzed under various contents of anions in molten salt. Then, the complexation behaviors and mechanisms of Ti-F/O were obtained for the purpose of optimizing the composition of electrolytes. The electrochemical behaviors of the complexes were discussed for clarifying the influence of anions on kinetics mechanisms of the electrolysis process and the properties of the molten salt. A quantitative method for estimating oxygen content was also offered. The paper would provide a better understanding mechanisms of kinetics of high pure titanium electrolysis, and the basic theory and experimental data can be used for reference in the industrialization process.

Keywords: Molten salt, integrated circuit, titanium, electrorefining

FA-P13

Metallurgical Performances under Different Melt Feeding Modes in a Bloom Continuous Casting Mould

Haibo Sun[1], Zheng Li[1], Liejun Li[2], Dongchu Chen[1]

1.Foshan University

2.South China University of Technology

Objectives: The metallurgical behaviors of melt flow, heat and mass transfer in the mould cavity were numerically analyzed upon the respective adoption of conventional straight single and bilateral-port nozzle, and a new type of swirling flow nozzle for bloom continuous casting (CC) process equipped with in-mould electromagnetic stirring (M-EMS).

Methods: For this purpose, a coupled model of electromagnetism, heat and solute transport were developed, and the corresponding plant trials were conducted in Shaoguan Steel, China.

Results: An alternate stirring mode can be formed in the mould cavity under the condition of SFN plus with M-EMS, where a swirling flow in the anti-clockwise direction generated by SFN and the other swirling flow in the clockwise direction induced by M-EMS are observed at the regions with distances ranging from 0m to 0.11m and 0.218m to 1.4m from meniscus, respectively. It is shown that the alternate stirring mode in the mould region can promote the superheat dissipation of molten steel, move the hot spot upward, inhibit the mould level fluctuation, which can be beneficial to improving the casting soundness and componential homogeneity and prevention of the slag erosion for the nozzle wall at the meniscus. Meanwhile, the melt temperature near the free surface can be increased by 2.0 K to 3.6 K, and the magnitude of mould level fluctuation is reduced from 5.6mm to 2.3mm as compared with the two other normal nozzles.

Conclusions: The alternate stirring mode generated by SFN plus with M-EMS is the easiest way to further enhance the metallurgical effect of M-EMS without investment of additional facilities for CC process.

Keywords: Bloom continuous casting, Mould metallurgical behaviors, numerical simulation, swirling flow

FA-P14

Atom-Resolved Observation of Au Dendrites Evolved from Nanoparticles on MoS_2

Yinghui Sun[1], Haofei Zhao[1], Dan Zhou[2], Rongming Wang[1]
1.University of Science and Technology Beijing
2.Stuttgart Center for Electron Microscopy, Max Planck Institute for Solid State Research

The morphology and structure stability of the interfaces of metal nanoparticles/2D semiconductors are of great importance for nano-devices. Au nanoparticles (NPs) with optimized size and distribution were deposited on few-layer of MoS_2 by e-beam evaporation. Epitaxial alignment between the metal NPs and 2D semiconductors was observed by the formation of Au dendrites on MoS_2 after the sample placed in the protection of dry N_2 for several days at room temperature. The morphology and structure evolution of the Au NPs/MoS_2 was investigated by atom-resolved microscopy characterization and quantitative simulation. Epitaxial alignment between the metal and MoS_2 can be accelerated by the high energy electron beam. Atom-resolved dynamic TEM and STEM investigation indicates that the metal atoms with low coordination number tend to migrate to the substrate by the interaction of electron beam and the particle, which paves a channel to merge the nearby NPs together and forms dendritic structures. Detailed characterization reveals that the Au dendrites were epitaxially grown on MoS_2 with lower energy. The long-range alignment of Au dendrites could give rise to improved current injection at the interface of metal and 2D semiconductors.

Keywords: Au nanoparticles, MoS_2, Au dendrites, STEM

FA-P15

高效准固态量子点敏化太阳能电池研究

卫会云[1,2]，郑新和[1]，李冬梅[2]，孟庆波[2]
1.北京科技大学
2.中国科学院物理研究所

量子点敏化太阳能电池（QDSCs）作为第三代太阳能电池，因量子点本身独特的光电学性质而被广泛研究，尤其是近年得到快速发展。为了进一步提高 QDSCs 光电转换效率以及改善电池界面载流子传输，我们首次将气相 SiO_2 纳米颗粒引入到 CdSeTe QDSCs 的多硫电解液来调控 TiO_2/CdSeTe/电解液界面，与传统的凝胶电解质不同的是，基于 SiO_2 复合电解液的 CdSeTe QDSCs 获得更高的填充因子和开路电压，电池性能被显著提高，同时电池的稳定性得到改善。我们进一步对 SiO_2 复合电解液基 CdSeTe QDSCs 的电子传输和复合过程进行了系统研究，研究表明，SiO2 纳米颗粒沉积在 TiO_2 和量子点表面形成能级势垒有效阻止了量子点和 TiO2 中电子向电解液的注入，从而有效减少了光生电子的复合；此外，基于 SiO_2 复合电解液的 CdSeTe QDSCs 具有更高的电子收集效率（98%）和更长的电子寿命。11.23%的光电转换效率以及 11.3%的认证效率也是目前液结 QDSCs 的最高效率之一。本工作为改善 TiO2/量子点/电解液界面提供了一种简便有效的方法。

关键词：量子点敏化太阳能电池；气相 SiO_2 纳米颗粒；准固态；高效率；载流子传输

FA-P16

Study on Microstructures and Properties of Spinning for Silicon Carbide Particle Reinforced Aluminum Composite

Haibao Wu[1], Defu Li[2], Guoqiang Chai[2], Jizhen Li[1], Degui Liu[1]
1.Aviation Industry Corporation of China Manufacturing Technology Institute
2.General Research Institute for Nonferrous Metals Beijing

In this paper, 15% SiCp/2009A1 composites were subjected to multi-pass hot spinning experiments. The principle of the microstructure and properties of the materials was studied with the increase of thinning rate. The microstructures, interfaces, precipitates and their properties of the tube, which were in the states of spinning, spinning and solution heat treatment were analyzed and discussed.

The research shows that it is possible to prepare spinning pipe with good shape and smooth surface by taking use of the spinning process of this paper. During the power spinning process, the force of the rotary wheel to the pipe causes the billet to produce two-way deformation, and the axial and tangential grains are obviously elongated and the flow line is formed.

There are mainly Al, SiC, $CuAl_2$ and Mg_2Si phases in the tube, and the spinning deformation does not change the phase composition of the composites, but the SiC distribution can be more uniform and the oxide film on the surface of the aluminum particles is broken, as a result that the oxygen element will cluster at the interface. After solution heat treatment, $CuAl_2$ and Mg_2Si dissolved, Cu evenly distributed in the matrix, but a small amount of Mg is still segregation in the grain boundary and SiC and aluminum matrix interface.

The solution heat treatment after spinning can greatly improve the yield strength and tensile strength of SiC/Al composites with a slight decrease in plasticity. The spinning process used in this paper can not only form a composite pipe with a smaller diameter and thinner wall thickness, but it can still be applied when the diameter of the pipe blank becomes larger and the wall thickness becomes thicker.

Through the research on spinning process and microstructure, the feasibility of spinning process for preparing aluminum matrix composites pipes was explored, which provided technical and theoretical support for the preparation and processing of Particulate reinforced aluminum matrix composites (PRAMCs) pipes for aviation and aerospace applications.

Keywords: Particle reinforced aluminum matrix composites, Spinning, Process Line, Microstructure, Interface

FA-P17

Lubrication and Surface Quality Control of Aluminum Strips in Hot Rolling Process

Lei Xia[1], Yan Li[2,3], Hongmei Zhang[4]

1.Research Institute of Petroleum Processing, SINOPEC

2.State Key Laboratory of Metal Material for Marine Equipment and Application

3.Iron & Steel Research Institutes of Ansteel Group Corporation

4.University of Science and Technology Liaoning

Aims. Energy saving and enhancing productivity have always been the theme in the modern industrial production. The surface quality of aluminum strips is increasingly strict especially in the hot rolling process because of the hereditary of rolling defects. To achieve the above aims, lubrication technology is an effective measure. Lubrication technology is essential in the production of aluminum strip and the lubrication effect is closely related to the quality of lubricant. This paper aimed to investigate the reason for the difference in the lubrication effect and surface quality of the rolled surface under various lubrication conditions and seek out effective parameters to choose a proper lubricant.

Methods. In the paper, 3104 aluminum alloy strips were selected and rolled by two rollers reversible hot rolling test unit. Two emulsions (SP-1 and SP-2) were employed respectively in the rolling process comparing with the condition of without lubrication. The thickness of work piece and the rolling force of each rolling pass were collected. The surface profile and microtopography of the rolled surface were observed by surface profiler and microscope. The tribological properties and wettability of emulsions were characterized as well.

Results. The results showed that lubrication technology could decrease the minimum thickness of rolled strips by 3.25 percent to 28.0 percent, reduce the rolling force by 36.8 percent to 39.7 percent and improve the quality of the rolled aluminum surface. The lubrication effect of SP-2 and surface quality of aluminum strip lubricated by SP-2 was superior to that of SP-1. The wetting angles of SP-1 and SP-2 were 51.6°and 40.8°, respectively. As for tribological properties, the maximum non-seizure loads (PB) of both SP-1 and SP-2 reached 735N. However, the friction coefficient (μ) of SP-1 was 0.124 and the wear scar diameter (D) was 0.56mm while the μ and D of SP-2 were separately 0.108 and 0.52mm.

Conclusions. The excellent wettability of SP-2 makes it spread out in the surface more quickly, form oil film and achieve the effect of lubrication. The lower μ of SP-2 could reduce the friction more effectively in the rolling process which is useful for decreasing rolling force and saving energy. The more inferior D of SP-2 explained that it could reduce wear in the rolling process which is beneficial to improve the surface quality of aluminum strip. Lubrication technology could increase the rolling reduction,

reduce rolling passes and improve the productivity of rolling mill. However, the effect of various lubricants is extremely different. The wetting angles, μ and D may be effective parameters to select an excellent lubricant, obtain excellent lubrication effect and improve the quality of rolled surface.

Keywords: hot rolling; lubrication; surface quality; energy-saving

FA-P18

Studies on Thermal-stress Response of Ni-base Alloy Coating with Energy Addition

Li Zhang
Institute of Fluid Physics, CAEP

Aims: Ni base alloy is of good heat-resisting ability, it is mostly applied in the engine of airplane, the turbojet and the nuclear reactor, so its thermal fatigue damage cannot be avoided. Ni base alloy ceramic composite coating is a mechanic disordered composite; a large number of ceramic particles are distributed in ductile matrix. The experiments show that cracks produce mostly between ceramic particles and Ni base alloy matrix and grow mostly along boundary of phases. Because the thermal expansion coefficients and elastic modulus of Ni base alloy and ceramic particles are different, there will be thermal stresses in both particles and matrix in thermo syphon process. There will be the strange stress and strain field between particles and matrix, so crack easily produces and grows.

Methods: Finite element model of Ni-base alloy coating under laser irradiation was constituted based on computational fluid dynamics (CFD) and computational structural dynamics coupling numerical computational methodology. The flow is governed by the 3-D Reynolds averaged Navier-Stokes equations. To split the viscosity flux and the convective flux of the NS equations, the second order central scheme and the ROE scheme were adopted respectively. With the implicit Gauss-Seidel scheme, the code was advanced in time. The turbulence model was used for turbulence simulations.

Results: Ni-base alloy coating of aircraft which are irradiated by laser are simulated. The model was proofread with the experiment data in atmosphere condition.

FA-P19

Technical Study on Preparation of Co/C Composite Nanofibers via Electrospinning

Sa Zhang, Jianjiang Wang, Fang Zhao
Army Engineering University Shijiazhuang Campus

Co/C composite nanofibers are prepared through electrospinning. Effect of Spinning humidity, salt and receiving equipment on composite fiber morphology were investigated. The morphology of composite fibers was observed by scanning electron microscopy (SEM).It was found out that when the ambient humidity was high, the nanofibers were agglomerated into fiber bundles. When the roller receiving equipment was used, ordered nanofibers can be obtained. Only cobalt acetate-doped composite nanofibers maintained intact fiber morphology after pre-oxidation and carbonization. And Co^{2+} was completely reduced to face-centered cubic structured Co nanoparticle. The ideal preparation technology is as follows: the humidity at 30% or less, doping with organic salt of cobalt acetate.

Keywords: electrospinning; composite nanofibers; Co nanoparticle

FA-P20

Near-Infrared Waveguide Formation and Surface Damage Analysis in LiF Crustals via Ion Irradiation

Lian Zhang
Taishan University

We report on the fabrication of waveguide structures in LiF crystals by 6.0 MeV with the different fluence carbon ions implantation at room temperature. The guiding modes were measured by the prism-coupling method at the wavelength of 632.8 nm and 1539 nm. The near-field intensity distributions of the sample with the maximum fluence were obtained by the end-face coupling method, and the simulation of the light propagation process was performed simultaneously for comparison. The waveguide characteristics were investigated in the near-infrared bands. The propagation loss of the waveguide was estimated to be 1.3 dB/cm. The damage profiles in the near-surface of the irradiated regions can be analyzed based on displacements per atom calculation using the SRIM code.

Keywords: planar waveguide, LiF crystal, ion irradiation

FA-P21

Research on Influence of Interference Fit on Fatigue Life of 2024-T351 Aluminum Alloy Double Shear Lap Joints

Qingyun Zhao[1], Hong Huang[1], Yunliang Wang[2]
1.AVIC Manufacturing Technology Institute
2.Naval Aeronautical Engineering Institute

Double shear lap joints were manufactured with hi-bolt interference fit and material of joints was 2024-T351 Aluminum alloy . Fatigue tests were carried out with different interference joints and also analized by FE simulation. Interference values range from zero clearance to 0.05,0.08,0.11 and 0.14. The results show that fatigue life is affected by levels of interference and interference fit is benefit for improving fatigue life. The residual stress distribution gained from FE simulation help to explain fatigue crack initiation and the trends of fatigue lives. There is good agreement between the numerically predicted fatigue lives and experimental fatigue test results.

Keywords: interference fit, fatigue life, double shear lap joints, FE, residual stress, fastener

FA-P22

Tailorable Shell Thickness in Monodisperse Cu@Ag Core-Shell Nanocrystals

Xiyue Zhu
Beijing Institute of Technology

The synthesis of monodisperse Cu and Ag bimetallic noble mental nanocrystals are reported. Using inorganic mental salts as precursors, highly monodisperse Cu and Cu@Ag core-shell nanocrystals(NCs) were synthesized at low temperature (~60 ℃) via a successive reduction process. The synthesis of Cu@Ag core-shell NCs with different shell thickness was realized by controlling the amount of precursors, whose diameter ranged from 10 to 14 nm. HRTEM, XPS and XRD analytical techniques were applied for the morphologic and structural analysis of Cu@Ag core-shell NCs. The XRD indicates the Cu core and Ag shell are face-centred cubic structure. UV-vis-NIR spectra of Cu@Ag colloidal dispersion displays two band corresponding to the LSPR of Cu and Ag, and the Cu band shifted to higher energy. This result forebodes this structure noble mental has a potential application in catalysis.

Keywords: Cu@Ag core-shell; nanocrystals; synthesis; different shell thickness

仅发表论文

FA-PO-01

Architecture Design of III-Nitride Semiconductors and Devices for Optical, Mechanical, Humidity Sensing

Mingzeng Peng, Xinhe Zheng, Sanjie Liu, Huiyun Wei, Yingfeng He, Meiling Li, Yunlai An, Yimeng Song, Peng Qiu
University of Science and Technology Beijing

Smart sensing becomes a key technological and economic driver for global industries with wide range of applications in internet of things, environmental monitoring, health care, infrastructure monitoring, national security, and so on. As important optoelectronic semiconductors, III-Nitrides are highly desirable for robust solid-state sensors capable of optical, gas, chemical/biological, humidity, mechanical sensing and pressure imaging especially in harsh environments. By architecture design, we have developed several low-dimensional microstructures and related functional devices for Nitride-based multifunctional sensing and single-chip integration, based on the transferrable vertical GaN nanowire array, well-guided horizontal GaN nanowire array and flexible GaN membrane. The multi-field coupling sensing effect has been proposed and further utilized for performance enhancement of optical, mechanical and gas sensing. It may provide a universal way for highly sensitive applications.