A02-纳米材料与新能源

A02-Nanomaterials and New Energy

分会主席：麦立强、张加涛、彭海琳、张桥

A02-01

A Cut-and-paste Approach to 3D Graphene Oxide-based Architectures

Jiaxing Huang
Northwestern University

Properly cut sheets can be converted into complex three-dimensional (3D) structures by three basic operations including folding, bending and pasting to render new functions. Folding and bending have been extensively employed in crumpling, origami and pop-up fabrications for 3D structures. Pasting joins different parts of a material together, and can create new geometries that are fundamentally unattainable by folding and bending. However, it has been much less explored, likely due to limited choice of weldable thin film materials and residue-free glues. Here we show that graphene oxide (GO) paper is one such suitable material. Stacked GO sheets can be readily loosened up and even re-dispersed in water, which upon drying, re-stack to form solid structures. Therefore, water can be utilized to heal local damages, glue separated pieces, and release internal stress in bent GO papers to fix their shapes. Complex and dynamic 3D GO architectures can thus be fabricated by a cut-and-paste approach, which is also applicable to GO based hybrid with carbon nanotubes or clay sheets.

A02-02

LDH Married to Carbon Materials to Create Novel Hybrids for Supercapacitors

Jieshan Qiu
1. School of Chemical Engineering, State Key Lab of Fine Chemicals, Liaoning Key Lab for Energy Materials & Chemical Engineering, Dalian University of Technology, China
2. College of Chemical Engineering,Beijing University of Chemical Technology, Beijing, China
* Email: jqiu@dlut.edu.cn; qiujs@mail.buct.edu.cn

For the high performance energy storage and conversion systems, such as pseudocapacitors, metal-air batteries, and electrocatalytic splitting water devices, one key issue is to tune the surface electrochemical reactions in the systems where multi-ions and multi-electrons transfer are usually involved. It is known that the reaction kinetics severely limits the efficiency of the energy storage and conversion devices, yet, how to tackle this bottle-neck issue remains a challenge. One powerful approach is to design and fabricate 3D functional carbon-based electrode materials with turned nanostructure that can speed up the reaction kinetics. Herein, we report the synthesis of transition metal layered double hydroxides (LDH)-carbon nanohybrid electrodes made of NiCoAl-LDH and various nano-structured carbon materials, including 0D carbon black (CB), 1D carbon nanotubes (CNTs), 2D reduced graphene oxide (RGO), and 3D CNT/RGO composites for pseudocapacitors. We tried to understand the role of the nanostructured carbon materials in terms of the pore structure and electrical conductivity as well as electrochemical reaction kinetics. To further improve the reaction kinetics of electrode materials and improve the specific capacitance and energy density of supercapacitors, we fabricated a flexible 3D architecture electrode made of NiCoAl-LDH nanoplates coupled with NiCo-carbonate hydroxide (NiCo-CH) nanowires, grown on ultralight carbon film (graphite paper, GP) by an in situ one-step hydrothermal method. The nanowire-like NiCo-CH species in the nanoplate matrix function as a scaffold and support the dispersion of the NiCoAl-LDH nanoplates, resulting in a relatively loose and open structure within the electrode matrix. The 3D architecture electrodes rich of electroactive species help to enhance the total specific capacitance, and to improve ions/charge transport due to the large interfacial area. Asymmetric supercapacitors have been fabricated with the nanohybrid as the positive electrode and a activated carbon (AC) as negative electrode, showing a high energy density of 58.9 Wh kg^{-1} at a power density of 0.4 kW kg^{-1}. Inspired by the nanowire-like species acting as scaffold and support in the 2D nanosheet matrix, we further developed a new strategy for graphene oxides (GO)-induced ultrafast self-assembly of monolithic NiCo-carbonate hydroxide (NiCo-CH) nanowire composites (G-CH). The oxygen functional groups on the GO surface help to effectively induce the formation of the monodisperse NiCo-CH nanowires. The G-CH composite films show a high volumetric density, superior volumetric capacitance, and excellent cycle life. A simple strategy to fabricate edge site-enriched nickel-cobalt sulfide (Ni-Co-S) nanoparticles decorated on graphene to make integrated hybrid architectures (Ni-Co-S/G) via in-situ chemical conversion method is also developed, where the Kirkendall effect is involved via anion exchange reaction, and the etching effects of the S^{2-} ions, plays a crucial role for forming the edge site-enriched nanostructure. The Ni-Co-S edge sites show high electrochemical activity and strong affinity for OH^- in the electrolyte. The asymmetric supercapacitor made with the edge site-rich Ni-Co-S/G hybrids as the positive electrode and 3D porous carbon nanosheets as negative electrode showed a high energy density of 43.3 W h kg^{-1} at a power density of 0.8 kW kg^{-1}, and an energy density of 28.4 W h kg^{-1} can be retained even at a high power density of 22.1 kW kg^{-1}.

Our work has shown that the 3D functional architectures made of carbon and pseudocapacitive species with enhanced reaction kinetics are of great potential as electrodes for supercapacitors. This also helps to shed a new light on the design of carbon-based electrode materials for energy storage.

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A02-03

Raman spectroscopy of two-dimensional semiconductor materials and related heterostructures

Pingheng Tan*
Institute of Semiconductors, Chinese Academy of Sciences

Two-dimensional materials (2DMs), such as graphene and transition metal dichalcogenides (TMDs), have been under intensive investigation. The rapid progress of research on graphene and TMDs is now stimulating the exploration of different types of 2DMs. The atoms within each layer in 2DMs are joined together by covalent bonds, while van der Waals interactions keep the layers together to form multilayer 2DMs, which makes the physical and chemical properties of 2DMs strongly dependent on their thickness (or layer numbers). These various 2DMs could be re-stacked/assembled horizontally or vertically in a chosen sequence to form van der Waals heterostructures (vdWHs), which can offer huge opportunities for designing the functionalities of such heterostructures. Two or more 2DMs with similar properties can be alloyed into a new type of 2DMs, namely, 2D alloy, which can offer tunable band gaps for promising applications in nanoelectronics and optoelectronics. Except the isotropic 2DMs such as graphene and 2H TMDs, anisotropic 2DMs such as black phosphorus (BP), SnSe, rhenium disulfide and rhenium diselenide (ReSe2) have one more degree of freedom to deliver various physical properties.

Raman spectroscopy is becoming increasingly important in the area of 2DMs. Raman spectroscopy can reveal information on the crystal structure, electronic structure, lattice vibrations and flake thickness of 2DMs, and can be used to probe the strain, stability, charger transfer, stoichiometry, and stacking orders of 2DMs. In particular, the unique interlayer vibrations have been widely used to develop a substrate-free layer-number identification of 2DMs, and to probe the strength of interlayer coupling in 2DMs and the interface coupling in artificial vdWHs. Here, we will review the recent advances on Raman spectroscopy in the characterization of different kinds of 2DMs and the corresponding 2D alloy and vdWHs. We will show that Raman spectroscopy is an ideal tool to probe the fundamental physics and potential applications of these various 2DMs, particularly when they are reduced down to monolayers or multilayers.

Keywords: Two-dimensional materials, nanoribbon, nanocrystals, Raman spectroscopy, interlayer coupling

A02-04

Construction and electrochemical energy storage of inorganic mesoscopic-scale assembly structure

Shenglin Xiong
Shandong University

The applicant has mainly engaged in the fundamental research of inorganic material chemistry. By direction of functionalization of energy storage, he has made the following important progress in inorganic mesoscopic scale materials: 1) the applicant establishes novel controllable preparation methods towards carbon-based mesoscopic scale composites. Importantly, by optimizing the surface structure and electronic structure of their active site, the energy storage property is greatly improved; 2) the applicant realizes the controllable synthesis and performance optimization of 3d electron mixed transition-metal oxide mesoscopic structures by regulating the nonequilibrium kinetic reaction process. 3) Taking the application as the direction, the applicant realizes the scalable preparation of high-performance carbon-based materials, which lays the foundation for the application of inorganic materials in energy storage.

Keywords: nanocomposite chemistry; controllable preparation; synthetic methodology; energy storage

A02-05

Chloride-passivated Mg doped ZnO nanoparticles for improving the performance of cadimum-free quantum-dots light-emitting diodes

Fei Chen*[1,2], Zhenyang Liu[1,2], Zhongyuan Guan[1], Zhenbo Deng[2], Feng Teng[2], Aiwei Tang[1,2]
1. Key Laboratory of Luminescence and Optical Information Beijing Jiaotong University
2. School of Science Beijing JiaoTong University

Much progress has been made in the improvement of the device performance of quantum dots light-emitting didoes (QD-LEDs) in the past few decades, most of which were mainly focused on the cadimum-based semiconductor QDs. However, the presence of the heavy metals in the QD-LEDs limits their further commercialization. As a result, some cadimum-free semiconductor nanocrystals have been developed, in which multinary cooper-based semiconductor nanocrystals have attracted much attention due to their low toxicity, high absorption coefficients and earth-abundant. Unfortunately, the performance of QD-LEDs based copper-based nanocrystals still falls behind that of cadimum-based QD-LEDs. A lot of work was reported to improve the device performance by optimizing the nanostructures of materials and device architectures. Among different approaches of device architectures optimization, interfacial engineering is one of the most popular and effective methods to improve device performances of cadimum-free QD-LEDs. In our previous work, red, yellow and green-colored QD-LEDs based on Cu-In-Zn-S/ZnS nanocrystals were reported using a solution-processed method, in which the colloidal ZnO nanoparticles were incorporated into the devices as an electron-tranportating layer. By optimizing the device fabrication process, the maximum external quantum efficiency (η_{EQE}) of yellow QD-LEDs could reach up to 2.4%. In this work, a systematical study of Mg doped ZnO (ZnO:Mg) nanoparicles as an electron-transporting layer in cadimum-free QD-LEDs indicates that the ZnO:Mg nanoparticles exhibit a favorable band alignment with the Cu-In-Zn-S/ZnS nanoparticles, which could help the electron injection from cathode layer to the emitting layer. As a result, the maximum η_{EQE} of the QD-LEDs is nearly twice as high as that of QD-LEDs using ZnO nanoparticles as the electron-transporting layer. Moreover, Sargent et al demonstrated chloride-passivated ZnO (Cl@ZnO) nanoparticles could reduce the surface defect sites and a favorable electronic band alignment, and thus the performance of the colloidal quantum dot photovoltaic devices could be improved greatly. Inspired by the study, we also employed Cl@ZnO nanoparticles as an electron-transporting layer in QD-LEDs, and the maximum η_{EQE} is very close to the device using Zn:Mg nanoparticles as an electron-transporting layer. Furthermore, we combine the advantages of both ZnO:Mg and Cl@ZnO nanoparticles to synthesize Cl@ZnO:Mg nanaoparticles, which are used as an electron-transporting layer to fabricate QD-LEDs based on Cu-In-Zn-S/ZnS nanocrystals, and thus the maximum η_{EQE} can be enhanced to 3.72%, corresponding to maximum current efficiency (η_A) of 11.1 cd A^{-1}. By varying the amount of Cl sources in the synthesis of Cl@ZnO:Mg, the maximum η_{EQE} of the device could be enhanced from 3.72 to 4.05% with an increase of Cl amount from 0.1 to 0.3 mmol. However, further increasing the amount of Cl sources leads to a decrease of the device performance. The ultraviolet photoelectron spectroscopy (UPS) measurements and current-voltage characteristics of electron-only devices indicate that the Cl amount has an important effect on the band energy level and electron mobility and thus is beneficial to the electron injection and transport balance.

Keywords: QD-LEDs, Cadimum-free, Interfacial engineering, Cl@ZnO:Mg

A02-06

Biomimetic Asymmetric Nanochannel Membranes for Energy Conversion

Liping Wen*
Technical Institute of Physics and Chemistry, Chinese Academy of Sciences

Learning from nature has inspired the creation of intelligent devices to meet the increasing needs of the advanced community and also to better understand how to imitate biology.[1-3] As one of biomimetic nanodevices, nanochannels or nanopores aroused particular interest because of their potential applications in nanofluidic devices, biosensing, filtration, and energy conversions. Here, inspiration from biological ion channels in nature, we developed some biomimetic smart nanochannels and then applied those smart nanochannels in practical applications such as bioinspired photo-driven ion pump[4] and especially energy conversion.[5,6] By employing the biomimetic nanochannel membrane, we have developed a series of systems for gradient energy generation, which aims to harvesting the giant blue energy. Such applications with biomimetic nanochannels can not only help people to know and understand the living processes in nature, but also inspire scientists to study and develop novel nanodevices with better performance for the mankind.

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Keywords: biomimetic nanochannel; energy conversion; gradient energy generation

A02-07

Functional Transition Metal and Its Compound Nanomaterials：Controllable Synthesis, Structure Characterization and Physicochemical Properties

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

Energy and environmental problems have triggered an urgent need for sustainable clean energy and new energy storage/conversion devices. Transition metal and its compound nanomaterials, as catalysts for electrochemical reaction or electrode materials for energy storage, are feasible in science and potential in practical economic applications. Meanwhile, understanding the structure-property relationship of nanomaterials is also of great scientific importance. Precisely designing and tailoring the structural complexity, composition and surface chemistry at nanoscale are highly demanded to realize the high performance of energy storage/conversion materials. Recent years, our group has devoted much effort to improving the catalytic activity of Pt-based transition metal nanomaterials and exploring excellent pseudocapacitive Co-based transition metal compound nanomaterials. We have developed a convenient ultrasound-assisted synthetic strategy to densely and uniformly load Pt and Au nanocrystals on various supports (active carbon, graphene, and metal oxides). And we also have realized the layer-controlled synthesis of Pt-Ni nanostructures through an ambient aqueous method and obtained Pt-Ni double- and single-layered nanobowls. Both the Pt-Au/C catalysts and Pt-Ni nanobowls exhibit enhanced catalytic performance towards small organic molecule electro-oxidation. On the other hand, many transition metal compound nanomaterials with different morphology, composition and interface structure, such as hollow, channeled, and solid CoO nanoparticles, interconnected hierarchical Co_3O_4 and $NiCo_2O_4$ microspheres, CoO_x mesoporous microspheres, and Co_2P hollow nanoflowers, have also been successfully prepared via a solvothermal method and a thermal decomposition method. Employed as electrode materials for supercapacitors, they show component and structural dependent pseudocapacitive features. Using $NiCo_2O_4$, CoO_x and Co_2P as positive materials and active carbon or graphene as negative materials, we have fabricated several high-performance asymmetrical supercapacitors.

Keywords: Transition metal, Composite, Interface, Structure-property relationship

A02-08

Metal-organic Frameworks Based Materials for Energy Storage and Conversion

Guangqin Li*
Sun Yat-sen University

How to design and synthesize of efficient and earth-abundant catalysts for a wide variety of electrochemical energy storage and conversion reactions is a great challenge. Guided by the advantage of component manipulation, morphology control, and structure engineering, advanced MOF-based materials have exhibited remarkable activity, selectivity, and stability for various energy-conversion processes, manifesting great potential for replacing precious-metal-based catalysts in next-generation energy devices. We have studied MOF based materials (Pd@HKUST-1) for hydrogen storage[1]. Recently, we have synthesized a porous carbon nanomaterial loaded with cobalt nanoparticles (Co@NC-x/y) derived from pyrolysis of a Co/Zn bimetallic zeolitic imidazolite framework, which exhibits incredibly high activity as bifunctional oxygen catalysts[2]. For instance, the optimal catalyst of Co@NC-3/1 has the superb ORR activity with onset potential of ~1.15 V and half-wave potential of ~0.93 V. Moreover, its OER activity is better than commercial IrO_2 and it also presents a long-term stability for 2000 circles and a Tafel slope of 85 mV dec^{-1}.

Keywords: Metal-organic Frameworks, Energy Storage, Electrocatalyst

A02-09

Newly Designed Cycloplatinated Polymer Dots as Photocatalysts for Visible Light–Driven Hydrogen Evolution

HO-HSIU CHOU*
National Tsing Hua University

By mimicking natural photosynthesis, generating hydrogen through visible light–driven splitting of water would be an almost ideal process for converting abundant solar energy into a useable fuel in an environmentally friendly and high-energy-density manner. In a search for efficient photocatalysts that mimic such a function, here we describe a series of newly designed cycloplatinated polymer dots (Pdots), in which the platinum complex unit is pre-synthesized as a co-monomer and then covalently linked to a conjugated polymer backbone through Suzuki–Miyaura cross-coupling polymerization. Based on our design strategy, the hydrogen evolution rate (HER) of the cycloplatinated Pdots can be enhanced 12-times higher than that of pristine Pdots under otherwise identical conditions. Compared to the Pt complex blended-counterpart Pdots, the HER of cycloplatinated Pdots still exhibit over 2-times higher than that of physically blended one. Furthermore, the enhancement of the photocatalytic reaction time with high eventual hydrogen productions, and low efficiency roll-off are observed by utilizing the cycloplatinated Pdots as photocatalysts. Based on the exceptional performance, our cyclometallic Pdot systems appear to be a new type of promising photocatalysts for visible light–driven hydrogen evolution.

Keywords: Semiconducting polymers, Polymer dots, Photocatalysts, Visible light, Hydrogen evolution

A02-10

Energy Storage Mechanism in Aqueous Zinc-ion Battery

Jiang Zhou*
Central South University

Lithium-ion battery and sodium-ion battery have been applied in energy storage devices, but low safety factor owing to the active chemical properties of Li+ and Na+ encourage us to develop new battery chemistry. As a safe, cost-effective and pollution-free device, rechargeable aqueous zinc ion battery (ZIBs) shows desirable potential as an alternative to LIBs and SIBs, and it is considered to be more feasible for grid-scale applications. Recently, lots of work has been done to develop new cathode materials and zinc storage insights for rechargeable aqueous ZIBs. However, the proposed energy storage mechanisms in aqueous ZIBs are still complicated and unclear. In this talk, the crystal structure and electrochemical mechanism of some typical cathodes in aqueous ZIBs will be described. The relationship between the structure, composition, storage mechanism and the electrochemical properties will be discussed in detail.

Keywords: aqueous Zn-ion batteries, energy storage mechanism, high-rate capability, long-cycle life

A02-11

Atomic Layer Deposition of Transition Metal Sulfides and Its Applications in Energy Technology

Xinwei Wang*
Peking University Shenzhen Graduate School

Transition metal sulfides have recently aroused great attention for a variety of applications in energy conversion and storage devices. Many transition metal sulfides, such as cobalt, nickel, and iron sulfides, have shown superb electrochemical properties, so they are highly promising as candidate active materials for supercapacitors, batteries, and water-splitting electrocatalysis. Atomic layer deposition (ALD) is a well-known nanotechnology for preparing uniform, conformal coating films on complex 3D structures. Recently, ALD has gained particular attention in energy conversion and storage applications, as ALD has been demonstrated as an effective approach to uniformly and conformally load active materials onto complex 3D nanostructured electrodes. For most electrodes, their electrochemical properties are largely determined by the surface properties, and therefore conformally coating the surface by ALD is of particular importance for the device performance, as the optimization of the nanostructured geometry of the electrodes can be decoupled from the modification of the surface properties. On the other hand, however, ALD of metal sulfides is much less explored, as compared to oxides. The ALD processes for many of the important sulfides, such as CoS_x, NiS_x, and FeS_x, are still not well established, which therefore could seriously hinder their applications in energy devices.

Herein, we will present our recent progress on the ALD of CoS_x, NiS_x, and FeS_x. The metal sulfides were all deposited using metal amidinates as the metal precursors and H_2S as the sulfur source. The saturation behaviors of these ALD processes were carefully studied. Typical film properties, such as microstructure, purity, and morphology, were evaluated by various techniques including TEM, AFM, SEM, RBS, and XPS. With optimal deposition conditions, our ALD processes were able to produce high-quality, pure, smooth, and well-crystallized films of CoS_x, NiS_x, and FeS_x. In addition, all these sulfide films were able to uniformly and conformally cover deep narrow trenches with high aspect ratio of 10:1, which demonstrated the excellent conformality of our ALD processes.

We will also present a few examples to demonstrate the promising applications of these ALD sulfides in energy conversion and storage devices. ALD CoS_x showed excellent electrochemical redox kinetics in alkaline aqueous solution, and therefore it was a suitable candidate active material for supercapacitors. By conformally depositing CoS_x thin film on porous nickel foam electrodes, the synthesized ALD-coated electrodes showed remarkable supercapacitor performance with high specific capacitance, good rate performance, and good cycling stability. Meanwhile, ALD NiS_x was found to show excellent electrocatalytic performance toward OER, and therefore it was promising for electrocatalysis and metal-air batteries. Further studies showed that the ALD NiS_x converted to porous nickel oxyhydrate during electrochemical aging, and the aged product exhibited superior OER performance with good stability.

A02-12

A Rich Variety of Nanocrystals with Precise Controlled Dimensions, Compositions, and Architectures Enabled by Nonlinear Block Copolymers for Solar Cells, Photocatalysis, LEDs and Batteries

Zhiqun Lin
Georgia Institute of Technology, USA
Zhiqun.lin@mse.gatech.edu

A02-13

Smart Materials by Nanoscale Assembly

Yadong Yin
Department of Chemistry, University of California, Riverside

A02-14

Novel two-dimensional oxide/hydroxide nanosheets for energy storage

Linfeng Hu*, Yingchang Jiang, Zhichang Pan
Fudan University

Inorganic layered compound is an important functional material with characteristic layered crystal structure and exfoliation behavior, which have attracted considerable research interest in electrochemical energy storage devices owing to their intriguing surface effect and significantly decreased ion-diffusion pathway. Here we describe rationally designed metastable $CoSeO_3 \cdot H_2O$ (M-CSO) nanosheets synthesized by a facile hydrothermal method for use as a Li ion battery (LIB) anode. This crystalline nanosheet can be steadily converted into amorphous phase at the beginning of the first Li^+ discharge cycling, leading to ultrahigh reversible capacities of 1,100 and 515 mAh g^{-1} after 1, 000 cycles at a high rate of 3 and 10 A g^{-1}, respectively. The as-obtained amorphous structure experiences an isotropic stress which can significantly reduce the risk of fracture during electrochemical cycling.

Furthermore, we developed novel $ZnCo_{1.5}(OH)_{4.5}Cl_{0.5} \cdot 0.45H_2O$ nanosheets, the crystal structure of which was revealed by synchrotron X-ray powder diffraction data analysis. In-situ growth of $ZnCo_{1.5}(OH)_{4.5}Cl_{0.5} \cdot 0.45H_2O$ nanosheet arrays on conductive

Ni foam substrate was successfully realized. Asymmetric supercapacitors based on $ZnCo_{1.5}(OH)_{4.5}Cl_{0.5}·0.45H_2O$ nanosheets @Ni foam// PVA, KOH//reduced graphene oxide (rGO) exhibits a high energy density of 114.8 Wh kg^{-1} at an average power density of 643.8 W kg^{-1}. A foldable supercapacitor constructed from $ZnCo_{1.5}(OH)_{4.5}Cl_{0.5}·0.45H_2O$ nanosheets @ PET substrate shows excellent flexibility and mechanical stability. Our study developed novel layered oxide/hydroxide materials with unique crystal structure and superior electrochemical properties for energy storage devices.

Keywords: Layered compounds, crystal structure, energy storage, lithium ion battery, supercapacitor

A02-15

Engineering of active sites for efficient non-precious metal electrocatalysts

JinSong, Hu
Institute of Chemistry, Chinese Academy of Sciences

The increasing concerns on severe environmental issues and rapid fossil fuel depletion stimulate the intensive interests in renewable and sustainable energy sources. Fuel cells and electrochemical water splitting is considered as one of ideal options to feed energy demand without environmental concerns. The commercialization of these techniques requires the efficient, low-cost and durable electrocatalysts for oxygen reduction reaction (ORR), hydrogen evolution reaction (HER), and oxygen evolution reaction (OER).

The catalytic performance of these electrocatalysts are closely related to the intrinsic activity and the number of the accessible catalytic sites in the electrocatalysts. This presentation will focus on the exploration of earth-abundant efficient ORR, HER and OER electrocatalysts with an emphasis on the performance boosting by synergistically electronic and structural engineering. Several reasonable ways will be introduced for rationally engineering the morphological structure, electronic structure, and crystalline structure of electrocatalysts to augment the accessible catalytic sites and synergistically boost their intrinsic activity, thus leading to the significant performance enhancement of these low-cost materials for practical applications.[1-5] These results will open opportunities for the rational design and bottom-up synthesis of cost-effective and high-performance electrocatalysts for fuel cells and sustainable hydrogen production through electrochemical water splitting.

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A02-16

CO_2 to fuels through the electrochemical reduction

Jing Shen*[1],Marc Koper[2]
1. Hunan Institute of Engineering
2. Leiden University

CO_2 is the most notorious greenhouse gas, which has caused and will continue to cause climate change. The abundance of the CO_2 resulting from the excessive combustion of fossil fuels makes it a perfect raw material to produce valuable fuels. Among diverse methods, electrocatalytic reduction of CO_2 using renewable energies seems to be a promising long-term objective.Herein, we report on electrochemical reduction of CO_2 on a simple, cheap and commonly available molecular catalyst to 8-electron transferred product methane. The catalytic system is a pyrolytic graphite (PG) electrode coated with cobalt protoporphyrin (Co-PP), turning over CO_2 to methane in an aqueous acidic solution (pH=1-3) with a moderate overpotential (~ 0.5-1V). In the absence of buffer anions, the catalytic system shows higher activity and different selectivity. At pH=1, methane and H_2, which is a competing product, are the only gas products. The CO formation is observed at pH=2 together with the methane and H_2 as products. The most important aspect of the pH effect is that there is a potential range at which the CO and methane is formed while there is no sign of the formation of H_2. This means that we can control the selectivity of the electrochemical reduction of CO_2 by tuning the experimental conditions. The role of proton is understood by comparing the voltammetry of H_2 evolution reaction on Co-PP at different pH (1-3). Besides, in order to get an insight of the mechanism, electrochemical reduction of potential intermediates was also conducted.

Keywords: carbon dioxide, electrochemical reduction, methane

A02-17

Controlled Synthesis and Catalytic Studies of Energy Nanostructures: Active Sites Engineering and Bandgap Engineering

leyu wang*
Beijing University of Chemcial Technology

Exploration of efficient, stability and low-cost catalysts are crucial to the renewable energy conversion techniques, such as fuel cells, photocatalysis and photothermal ablation. We mainly focused on the precise control and delicate modulation of the microstructures of the nanomaterials to develop novel, high-performance nanocatalysts.

In terms of active sites engineering, we successfully synthesized ultrasmall Pd–Ni–P ternary nanoparticles for ethanol electrooxidation (Nat. Commun. **2017,** 8, 14136), which achieved the improved ethanol electrooxidation performance by shortening Pd–Ni active site distance. The activity is improved up to 4.95 A per mg Pd, which is 6.88 times higher than commercial Pd/C (0.72A per mgPd), by shortening the distance between Pd and Ni active sites, achieved through shape transformation from Pd/Ni–P heterodimers into Pd–Ni–P nanoparticles and tuning the Ni/Pd atomic ratio to 1:1. The improved activity and stability stems from the promoted production of free OH radicals (on Ni active sites) which facilitate the oxidative removal of carbonaceous poison and combination with CH_3CO radicals on adjacent Pd active sites. Additionally, we report a seed-growth strategy to synthesize ultrasmall donutshaped Cu_7S_4@MoS_2 heteronanoframes, fully exposing abundant, highly-active MoS_2 edge site for hydrogen evolution reaction. These nanoframes demonstrate an ultrahigh activity with 200 mA cm^{-2} current density at only 206 mV overpotential using a carbon-rod counter electrode，a Tafel slope of 48 mV/decade, and excellent stability over 5000 cycles in 0.5M of H_2SO_4 media (Angew. Chem.-Int. Edit. **2016,** 55, 6502; Small **2017,** 13, 1602235; Sci. China-Mater. **2017,** 60, 929; **2017,** 60, 352.).

In terms of bandgap engineering, we report a highly efficient photocatalyst comprised of Cu_7S_4@Pd heteronanostructures with plasmonic absorption in the near-infrared (NIR)-range (Nano Lett. **2015,** 15, 6295). The strong NIR plasmonic absorption of Cu_7S_4@Pd not only effectively boosted the sunlight utilization, but also facilitated hot carrier transfer from Cu_7S_4 to Pd, which subsequently promoted the photocatalytic reactions on Pd metallic surface, including the Suzuki coupling reaction, hydrogenation of nitrobenzene, and oxidation of benzyl alcohol. Even under irradiation at 1500 nm with low power density (0.45 W/cm^2), these heteronanostructures demonstrated excellent catalytic activities. Under solar illumination with power density as low as 40 mW/cm^2, nearly 80−100% of conversion was achieved within 2 h for all three types of organic reactions.We hope these findings will provide guidelines for the design and synthesis of novel efficient nanocatalysts.

Keywords: energy nanostructures, precise control, active sites engineering, bandgap engineering

A02-18

One-dimensional semiconducting nanostructures for flexible image sensors

Guozhen Shen*
Institute of Semiconductors, Chinese Academy of Sciences

Over the last few decades, advancements in flexible electronics have spread across an expansive area ranging from the development of fundamental transistors, different kinds of sensing devices, and flexible organic light-emitting diode displays in various kinds of flexible substrates. This academic interest in flexible electronics will continue for some years, which is driven by the growing demand for electronics permitting lightweight design, portability, and low manufacturing cost as compared to their rigid substrate counterparts, and supported by techniques for the ceaseless miniaturization of individual elements in microelectronics.

In this talk, I will briefly introduce some of the progress of flexible image sensors made of one-dimensional nanostructures in my group. Strategies to improve the performance of single nanowire devices were first introduced, including forming heterostructures, inorganic-organic hybrid nanostructures as well as nanowire arrays. Flexible image sensors are then fabricated with device arrays. By introducing metal oxide memristors, flexible artificial visual system was then developed.

A02-19

Negative/Zero Thermal Expansion in Black Phosphorus Nanotubes

Lei Wang*[1],Cong Wang[2],Qiang Gu[1]
1. University of Science and Technology Beijing
2. Beihang University

Black phosphorus nanotubes (BPNTs) as new one-dimensional materials have very promising prospects in nanoelectronics devices. Taking into account that the effect of finite temperature on nanoelectronic devices is indispensable, we perform a comprehensive first-principles study of thermal expansion of BPNTs. It is surprisingly found that the negative and zero thermal expansion behaviors can occur in BPNTs. The abnormal thermal expansion can be tunable by changing diameter and bonding in the unique configurations of armchair and zigzag BPNTs. In pristine BPNTs, the size effect appears in armchair nanotubes where the positive thermal expansion (PTE) is weakened generally with increasing diameter. In contrast, the thermal expansion of the zigzag nanotubes is diameter independent. Some zigzag nanotubes exhibit nearly zero thermal expansion (ZTE). For processed BPNTs with changed bonding, both types of nanotubes present negative thermal expansion (NTE) behavior. Differing from the diameter independence of NTE in processed zigzag nanotubes, the NTE in the processed armchair nanotubes is weakened gradually to nearly ZTE with increasing diameter. This work demonstrates that the special characteristics of edge shapes, size and bonding can play a crucial role in determining the abnormal thermal behaviors in BPNTs.

A02-20

High spatial resolution mapping of catalytic reactions on single nanoparticles

Elad Gross
The Hebrew University

The critical role of low-coordinated metal atoms in surface reactions and heterogeneous catalysis has been firmly established. But despite the growing availability of tools enabling detailed in situ characterization, it has so far not been possible to directly document this role: surface properties can be mapped with high spatial resolution and catalytic conversion can be documented with a clear chemical signature, but combination of the two, enabling high spatial resolution detection of chemical reactions on catalytic surfaces, was rarely achieved. Here we show that differently active regions within a given particle can be distinguished by mapping the chemical reactivity of N-Heterocyclic Carbene molecules (NHCs) attached to catalytic particles using synchrotron radiation-based infrared nanospectroscopy with a spatial resolution of 25 nm. It is demonstrated that compared to flat regions on top of the particles, the particles' periphery, containing low-coordinated metal atoms, is more active in catalyzing oxidation, as well as reduction, of chemically active groups in surface-anchored NHCs. These results indicate that high spatial resolution vibrational spectroscopy measurements can correlate between surface properties and reactivity, uncovering differences in reactivity between neighboring sites across the surface of single catalytic nanoparticles.

A02-21

Rational Design of Nanomaterials for Fuel Cell and Batteries

Shuhui Sun
Center for Energy, Materials and Telecommunications, Institut National de la Recherche Scientifique (INRS), Canada

A02-22

Design of nanotructured arrays electrodes for energy storage and conversion

Chuanwei Cheng
Tongji University

With the increasing concern over the global energy crisis and greenhouse effect by the carbon dioxide emissions, development of clean and sustainable energy solutions to the alternatives of traditional fossil fuels has attracted considerable interest.Nanostructured electrode are very critical for energy storage and conversion technologies including fuel cells, metal-air batteries,photoelectrochemical water splitting and electrocatalytic water electrolysis. The development of highly efficient and cost-effective electrode materials is highly desirable for the practical application of these technologies. In this text, I will introduce some of our research results about the design of arrayed electrodes including oxides based semiconductors, noble metals（Pt based materials）, non-precious transition metal oxide and sulfide materials for photoelectrocatalytic water splitting, methanol oxidation and Zn-air batteries applications.

A02-23

Nano-Materials for Hydrogen Storage and Rechargeable Batteries

Yu Zhang
Key Laboratory of Bio-Inspired Smart Interfacial, Science and Technology of Ministry of Education, School of Chemistry, Beihang University

Energy storage has been receiving great attentions for potential applications in electric vehicles and renewable energy systems. In this regard, fuel cells and rechargeable batteries have been proposed and intensively studied over past decades, wherein inorganic materials play a key and irreplaceable role to improve the energy efficiency and density. A flexible and wearable lithium–oxygen (air) battery inspired by Chinese bamboo slips is constructed. In this novel battery, cathodes and anodes are woven without an air diffusion layer and any outer packaging; besides, the woven structure allows oxygen to access the cathodes from both sides freely, endowing the battery with a record energy density of over 523 W h kg^{-1}. Novel integrated self-package flexible Li-O_2 battery is developed with a stable composite anode and flexible gas diffusion layer. Excellent mechanical stability and superior battery performances are successfully achieved under different shapes and even after repeated mechanical twisting, bending processes, showing high promise to power next generation versatile flexible electronics. In addition, superefficient water-splitting materials comprising sub-nanometric copper clusters and quasi-amorphous cobalt sulfide supported on copper foam are reported. While working together at both the anode and cathode sides of an alkaline electrolyzer, this material gives a catalytic output of overall water splitting comparable with the Pt/C-IrO_2-coupled electrolyzer. Furthermore, developing robust oxygen reduction electrocatalysts is still a critical challenge for the commercialization of fuel cells and metal-air batteries. Recently in Joule, Lin and colleagues constructed hollow porous spinel AB_2O_4 microspheres (A=Zn, B=Mn/Co) as efficient and durable oxygen reduction electrocatalysts and found the importance of the electronic transition of the spin state of Co^{3+} in boosting the catalytic performance. By harvesting the synergistic effect between the active component and the catalyst support, the influence of catalyst on the catalytic dehydrogenation performance of hydrous hydrazine has been systematically studied, and RhNi@graphene and noble-metal free Cu@Fe_5Ni_5 catalysts have been successfully obtained, which exert 100% H_2 selectively and exceedingly high activity to complete the decomposition reaction of hydrous hydrazine.

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Keywords: Lithium-oxygen batteries; Catalyst; Air cathode; Flexible devices

A02-24

高通量微纳加工及 3D 分析加工平台

高雪丽
蔡司（Zeiss）中国

A02-25

2D Oxide Nanomaterials and Their Superior Electrochemical Properties

Xudong Wang
University of Wisconsin-Madison
* Email: Xudong.wang@wisc.edu

Two-dimensional (2D) nanomaterials, particularly when their thickness is just one or a few atomic layers, exhibit physical properties dissimilar to those of their bulk counterparts and other forms of nanostructures. Nonetheless, 2D nanostructures so far have been largely limited to naturally layered materials, i.e. the van der Waals solids. A much larger and diverse portfolio of 2D materials including non-layered compounds are desirable to meet the specific requirements of individual components in various devices. We demonstrate that surfactant monolayers could serve as a soft template supporting the nucleation and growth of 2D nanomaterials in large area beyond the limitation of van der Waals solids. Through this approach, 1 to 2 nm thick, single-crystalline free-standing ZnO nanosheets with sizes up to tens of microns were synthesized at the water-air interface. This technique was denoted as the Ionic Layer Epitaxy (ILE) – the first solution-based technique for growing large-area ultrathin nanosheets without the support of crystalline substrates. ILE vastly broadens the range of 2D nanomaterials from layered van der Waals solids to oxide ceramics, opening up opportunities for discoveries of exciting transport, magnetic, photonic, and catalytic properties. So far, in addition to ZnO, we have showed successful synthesis results from CuO, CoO, MnO2, and Pd. The new 2D nanomaterials enabled by ILE will lead to extraordinary performance gain or new functionalities in many electrochemical disciplines, such as energy harvesting and storage, information systems, sensing, and optics.

A02-26

Controlled Preparation of Porous Nanomaterials for Energy Storage and Conversion by Tunable Self-assembly of Block Copolymers in Solution

Yiyong Mai*
Shanghai Jiao Tong University

Solution self-assembly of amphiphilic block copolymers provides a powerful bottom-up approach for the construction of supramolecular assemblies with tunable structures, which can be readily controlled by various factors including copolymer composition and concentration, the nature of solvent, the water content, etc.[1,2] Among diverse block copolymer assemblies, colloidal particles, e.g. polymer cubosomes consisting of inverse mesophases, have attracted considerable attention as they may serve as ideal platforms for porous materials with potential applications in, e.g. pharmaceutical sciences, chemical separation or energy-related devices.[3-10] In this presentation, we will discuss the tunable self-assembly of simple block copolymers, namely polystyrene-block-poly(ethylene oxide) (PS-b-PEO) diblocks, into porous cubosomes with inverse Im-3m or Pn-3m mesophase of controlled unit cell parameters as well as hexasomes with an inverse hexagonal (p6mm) structure (Figure 1), which have been rarely found in polymer self-assembly. A new morphological phase diagram for solution self-assembly of PS-b-PEO is plotted based on the volume fraction of the PS block against the initial copolymer concentration. The formation mechanisms of the cubosomes and hexasomes are revealed.[6]

Keywords: block copolymer, self-assembly, inverse mesophase, porous materials, supercapacitors,

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A02-27

Chirality-Related Applications of Helical Nanoparticles with Sub-10-nm Helical Pitches

Zhifeng Huang*
Hong Kong Baptist University

Metallic helices with a characteristic helical pitch (P) in the micro- or nano-scale have been proposed for diverse chirality-related primary applications. However, limit development of current nanofabrication techniques lead to P> 20 nm, so that molecules are too small in size to effectively perceive the helical chirality and the dimensional mismatch will substantially prohibit the development of those applications. In this talk, we will devise glancing angle deposition with fast substrate rotation to produce helical nanoparticles (hNPs) with sub-10-nm P, composed of controllable plasmonic materials and helicity. hNPs were employed to induce enantiospecific adsorption of molecules, mediate the enantiopreferential photocyclodimerization of 2-anthracenecarboxylic acid, and markedly enhance optical activity of chiral molecules. These studies will pave the way to developing hNPs for significant chirality-related applications, such as intrinsically chiral catalysts for heterogeneous asymmetric catalysis and determining absolute configuration of chiral molecules with high sensitivity.

Keywords: Helical nanoparticles; helical pitch; optical activity; photochirogenesis; enantiodifferentiation.

A02-28

Themally-enhanced generation of solar fuels

Liming Zhang[1*], Xiaofei Ye[2], Madhur Boloor[2], Nicolas A. Melsosh[2], William C. Chueh[2]
1. Department of Chemistry, Fudan University, 2005 Song-Hu Rd., Shanghai, China 200438
2. Department of Materials Science & Engineering, Stanford University, 946 Lomita Mall, Stanford, California, USA 94305

The extremely low carrier mobility in small-polaron semiconductors, such as $BiVO_4$, limits their photoactivity when being used as light absorbers in photoelectrochemical (PEC) devices. By increasing the temperature, the carrier mobility can be enhanced exponentially, providing an efficient strategy to improve the collection of minority carriers in the diffusion region. Here we explored the effect of elevated temperatures on the PEC properties of Mo-doped bismuth vanadate in buffered neutral aqueous electrolyte, highlighting the significant benefit of thermally activating carrier transport in polaronic light absorbers. We expect that our observation is general and will be applicable to other localized electron semiconductors. At last, we experimentally validate this thermal enhancement by developing a solid-state test platform and cell design to split water vapor into hydrogen and oxygen.

A02-29

Preparation of Modified Polyacrylonitrile Nanofiber Membranes and Application as an Adsorbent

Aiying Zhang*, Ning Gao, Guiyi Cao, Lin Ye, Zengguo Feng
Beijing Institute of Technology, School of Materials Science and Engineering

Heavy metal ions such as copper, iron, lead, and chromium, have high toxic and nonbiodegradable properties. Generally, adsorption is regarded as an effective and economical method for the removal and recovery of heavy metal ions. The adsorption properties of adsorbents depend on the functional groups on their surfaces. Recently, the electrospinning technique has become a versatile approach for producing nanofibers with high surface area-to-volume and flexibility for chemical/physical functionalization. It has been found that an adsorbent containing nitrogen-based ligands is effective in forming complexation with metal ions. polyacrylonitrile (PAN) electrospinning nanofibers could be modified to contain a chelating group for the removal of metal ions. It is therefore of our interest to investigate the feasibility of using a nanofiber membranes modified with amine groups on its surface as an adsorbent of metal ions.

Firstly, PAN nanofiber membranes were successfully prepared by electrospinning of PAN/DMF solutions, then the PAN membranes were modified with amine oxime in the aqueous of hydroxylamine hydrochloride. These results showed that as the increase of reaction temperature, reaction time and the concentration of the hydroxylamine hydrochloride, the -CN conversion ratio also increased obviously, but accompanying with membranes size shrinking slightly and the membranes' color getting pale yellow. By combining with FTIR, SEM characterization, the optimum reaction conditions parameters were finally determined.

The adsorption effectiveness of Cu (Ⅱ), Pb (Ⅱ), Fe (Ⅲ) , after 10h equilibria were 35.8, 75.2, and 90.0mg/g, respectively. Results showed that Langmuir adsorption isotherm curve could fits well adsorption data of chelating fiber, and the coefficients were above 0.990, showing that the metal ion chelating nanofibers surface achieved monolayer adsorption. Adsorption process of chelating fiber on metal ion can be described by secondary dynamics equations, and kinetic studies have shown that oxime amine groups on metal ions adsorption processes were controlled by the diffusion of metal ions and coordination reaction. Adsorption and desorption of chelating fiber membrane on Cu (Ⅱ) experiments suggested that amine oxime PAN chelating fiber membrane can be facilely regenerated with hydrochloric acid solution.

Thus Amidoxime PAN chelating nanofibers could have a potential application in these areas of heavy metal ions pollution treatment, the enrichment and recovery of precious metals.

Keywords: Nanofiber, Electrospinning, Amidoxime, Adsorption

A02-30

Applications of Novel carbon materials and transition metal oxides/sulfides as electrode in flexible and wearable all-solid-state supercapacitors

Shanglong Peng*, Yuxiang Wen, Shuqi Lu
Lanzhou University

To further promote the practical applications of SCs and meet the booming development of novel electronics, our group has made some works to cater the demand by both taking full advantage of the merits of different electroactive materials and designing the configuration of electrode and device in the past 3 years. Firstly, 3D flexible O/N Co-doped graphene foam as supercapacitor electrode is demonstrated using both the superiority of high conductivity and mechanical property for graphene and the effect of heteroatoms doping to properties. With regard to the characteristic of excellent pseudo-capacity for transition oxides/sulfides, a series of electrodes are fabricated to further enhance performance of SCs such as MnO2 (nanoparticles), NiCo2S4 (ultrathin nano-petals), hybrid Co3O4/NiCo2O4. Under the background of rapid development of electronics, flexible and wearable all-solid-state supercapacitors with ultrahigh energy density based on a carbon fiber fabric electrode is designed and prepared as power source to drive the electronics such as watch and logo composed of many LEDs. Subsequent works in our group will continuously focus on the practical applications of SCs and dedicate self to promote the development of flexible and wearable electronics.

A02-31

Aerosol synthesis of crumpled graphene/tungsten disulfide/tungsten trioxide ternary nanohybrids as an efficient electrocatalyst for hydrogen evolution reaction

Yantao Chen*[1], Ren Ren[2], Mao Shun[3], Chen Junhong[2]
1.School of Materials Science and Engineering, Tianjin University of Technology
2.Department of Mechanical Engineering, University of Wisconsin-Milwaukee
3.State Key Laboratory of Pollution Control and Resources Reuse, College of Environmental Science and Engineering, Tongji University

Hydrogen is considered as a promising source of clean energy that could partially replace hydrocarbon fuels. There is a growing attention on hydrogen production from water splitting. Noble metals such as Pt-group metals, are most commonly used catalysts in the hydrogen evolution reaction (HER). Developing novel electrocatalysts for HER with both low-cost and high-performance is a challenge. Recently, both computational and experimental studies show that transition metal dichalcogenides (TMDs), i.e., molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2), are effective in catalyzing HER. The exposed edges of TMDs provide active sites for HER electrocatalysis while the basal plane is catalytically inert. The HER kinetics of TMD electrocatalysts are often sluggish because of the poor electrical conductivity. Carefully-selected catalyst support can prevent TMD nanostructures from agglomeration and improve the overall performance by facilitating the charge transfer. Graphene is a two-dimensional carbon material with one atom thickness. It has high specific surface area (~2,600 $m^2\ g^{-1}$) and electrical conductivity ($5\text{-}6.4\times10^6$ $S\ m^{-1}$) that are attractive for electrocatalyst support. It is noteworthy that graphene is also a soft material with a low bending rigidity and thus can be easily engineered with different morphologies. Crumpled graphene can provide extra benefits compared to the conventional graphene nanosheets, e.g., preventing the aggregation of graphene sheets and improving the contact between graphene and TMDs for an even more efficient electron transfer.

Herein, we fabricated the 3D crumpled graphene/WS_2/WO_3 hybrid (CGTH) nanostructure through the aerosolization of the mixture of graphene oxide (GO) suspension and ammonium tetrathiotungstate ($(NH_4)_2WS_4$). A brief (5 min) sonication was conducted on the mixed suspension for a better dispersion and ion adsorption. The as-prepared suspension was then aerosolized by an ultrasonic nebulizer (2.4 MHz). The aerosolized mist was carried by an inert gas (Argon, 1 L/min) and passed through a tube furnace preheated at 800 ^oC. The capillary force generated by the rapid evaporation of the solvent leads to the shrinkage of aerosol droplets and the compression of GO sheets. $(NH_4)_2WS_4$ in the aerosol droplets was thermally decomposed to WS_2 nanocrystals, while the nanocrystals were encapsulated by the thermally reduced GO (rGO) sheets. WS_2 can react with water vapor under high temperature, so WS_2 can be partially converted to WO_3. The as-produced hybrid materials were collected by a Teflon filter at the exhaust of the tube furnace for further analysis.

The scanning electron microscopy (SEM) characterization reveals that the CGTH has a size distribution from 200 to 800 nm with a 3D crumpled structure and the rod-like nanocrystals are decorated on the rGO sheets. The energy-dispersive X-ray spectroscopy (EDS) characterization shows that oxygen element has a higher intensity around the edge of the encapsulated nanorods, indicating the quasi core-shell structure between WS_2 and WO_3. The X-ray diffraction (XRD) patterns and Raman spectrum further confirm the coexistence of rGO, WS_2 and WO_3, which is in good agreement with the selected area electron diffraction (SAED) results. To investigate the surface area and porous structure of CGTH, nitrogen adsorption-desorption isotherm curves were measured and identified as type IV. CGTH has a specific surface area as ~ 18 $m^2 g^{-1}$, with adsorption average pore width ~129.3 Å.

The HER activity of CGTH was characterized by depositing the as-prepared materials on a glassy carbon electrode and testing in a 0.5 M H_2SO_4 solution using a three-electrode setup. As a reference, a commercial Pt/C catalyst was used for comparison, which exhibited a nearly 0 V onset overpotential. The polarization curve recorded with CGTH on glassy carbon electrodes shows a small onset overpotential of 96 mV, which is comparable to that of Pt and implies low energy consumption in the catalytic process. The overpotential required to drive the current density of 10 mA cm^{-2} for CGTH is determined as 113 mV. Tafel slope is an inherent property of catalysts, which depends on the rate determining step (RDS). The Tafel slope for Volmer, Heyrovsky and Tafel reactions at room temperature are calculated as 120, 40 and 30 mV dec^{-1}. CGTH yields a very small Tafel slope of 37 mV dec^{-1}, suggesting the RDS for CGTH is Volmer-Heyrovsky mechanism. The observed small Tafel slope exhibited by CGTH can be attributed to the intimate contact between crumpled rGO and WS_2/WO_3 nanorods that results in a highly conductive system for facile electron transfer, which can be confirmed by the small charge transfer resistance derived from the Nyquist plot by electrochemical impedance spectroscopy (EIS). Meanwhile, CGTH shows a satisfying durability in the long-term electrolysis. The current retention of CGTH electrocatalyst after 15 hours' continuous operation was determined as 99.7%, implying the negligible activity decay.

Typically, TMD nanosheets were grown on the surface of two dimensional rGO, while the drawback was that the charge transfer was limited to two dimensions. Compared to the reported works on TMD/rGO-based electrocatalyst, CGTH has the advantage of 3D conductive network constructed by crumpled rGO for an even more efficient charge transfer. Previous studies of TMDs/rGO give the credit to strong chemical and electronic coupling between the rGO and TMDs with abundance of accessible edges that work as active sites in HER electrocatalysis. This study further verifies this theory and clearly demonstrates that crumpled rGO/WS_2/WO_3 ternary structure could serve as an even more efficient electrocatalyst for HER. With the excellent electrocatalytic activity, stability, and corrosion-resistance, CGTH could be a promising HER electrocatalyst to replace the precious Pt for water splitting application.

Keywords: crumpled graphene, tungsten disulfide, tungsten trioxide, nanohybrids, hydrogen evolution

A02-32

Controlling the electronic and optical properties of transition metal metal oxides by doping/defects for electronics and energy applications

Hongliang Zhang*, Gaoliang Fu, Jiaye Zhang
College of Chemistry and Chemical Engineering，Xiamen University

Metal oxides display a remarkable range of materials properties suitable for advanced electronics and clean-energy technologies. A fundamental understanding of the effect of defect/compositions on their electronic and catalytic properties is the key to advance this field, but is also a challenging task. The overall goal of our research is to address these issues using synchrotron-based photoemisson spectroscopic techniques (both XPS and x-ray absorption) to study the electronic properties of well-defined epitaxial thin films prepared by physical vapor methods. In this talk, I will use perovskite $LaCrO_3$ and NiO as examples to show the impact of oxygen vacancies (Vos) and dopants on their electronic and optical properties of significant implications for electronics and oxygen evolution reaction electrocatalyst. In particular, I will show aliovalent Sr doping in $LaCrO_3$ and Li doping in NiO introduces hole states at the top of valence band and the materials gradaully transit from a wide bandgap insulator, to p-type transparent semiconductor, due to hole state at the top of valence band of strong hybridized states of O 2p and Cr 3d or Ni 3d. We also found a fast oxide ion conduction at low temperature in SrCrO3-δ, which is of vital importance to the advancement of solid oxide fuel cel. Secondly, we also show Li doping can significantly enhance the oxygen evolution reaction activity of NiO. NiO is a wide bandgap (Eg=3.6 eV) semiconductor with eg2 configuration. Our results reveal a strong hybridization between O 2p and Ni 3d and more Ni^{3+} (eg1) state, leading to the remarkable enhancement of OER activity with Li doping. A new unoccupied state develops at 0.5 eV above the Fermi level, and dominates at higher Li level. This unoccupied state acts as the acceptor to facilitate a fast electron transfer from OH^- to the catalyst.

A02-33

Optical tuning of gold nanoparticle chains: from reversible assembly to interparticle gap engineering

Yiding Liu*
1. Department of Radiology, Xinqiao Hospital, Third Military Medical University
2. Department of Biomedical Materials Science, School of Biomedical Engineering. Third Military Medical University

Colloidal gold nanoparticles (AuNPs) possess unique optical properties originated from the localized surface plasmon resonance. Chain-like assembly structures of AuNPs exhibit distinct optical properties from individually dispersed AuNPs due to the plasmon coupling effect. Active tuning of optical properties of AuNPs and AuNP chains has been realized by development of strategies for reversible chain assembly as well as interparticle gap tuning in fixed AuNP chains. Both theoretical and experimental studies have revealed reversible assembly of AuNPs was governed by nanoparticle colloidal interactions while interparticle gap distance was able to be engineered by control of the surface ligand adsorption conditions. These strategies for active optical tuning have also been demonstrated to be useful in relevant applications.

A02-34

Mass-production of 3D graphene-like carbon for highly efficient solar thermal steam generation

Jinzhang Liu*, Lu Sun, Yan Li
Beihang University

Light absorbing materials that can efficiently utilize solar thermal energy to enable liquid-to-vapor phase transition of water are of great interest in technology and hold the potential to solve the long-standing water crisis. For practical application in clean water generation by using solar energy, the efficacy and cost of photothermal material have to be considered. Here, we report vapor-solid reaction method to produce 3D graphene-like carbon on a large scale by using Mg powder and CS_2 liquid as precursors. In a tube furnace, gram-scale carbon nanostructures are produced through Mg-reduction of CS_2 vapor at ~580 ^oC. The black carbon product is processed into hydrophilic membranes that generates steam at an efficiency of 92% under one sun, which surpasses most reported materials used in solar energy-driven water evaporation. When in air, the temperature of the carbon membrane surface reaches 105 ^oC under one sun, suggesting its efficient light-to-heat conversion ability.

A02-35

Rational design and controllable synthesis of nano-structured Cobalt-based electrocatalysts for oxygen evolution reaction

Fenglei Lv*, Qiao Zhang
Soochow University

Electrochemical water splitting and CO_2 reduction for the production of fuels and chemicals are widely considered as green technologies that can convert renewable energy into denser storing modes, i.e., chemical bonds. Oxygen evolution reaction (OER) plays a key role in providing the electrons and protons for the cathode reactions. Both IrO_2 and RuO_2 are well-known electrocatalysts because of their high activities and excellent kinetics for driving OER. However, high price and scarcity of the precious metals seriously hinder their widespread application.

Nano-structured Cobalt-based electrocatalysts have been proven to be a highly promising candidate, not only because of their relatively low price, but also their reasonable activities for OER. Nevertheless, the best known cobalt -based electrocatalysts still need a large overpotential to operate. In this presentation, I will start from our effort in the synthesis of two types of two-dimensional monometallic cobalt hydroxide nanoplates in aqueous solution for OER: α-$Co(OH)_2$ with both Co^{2+}Td and Co^{2+}Oh sites and β-$Co(OH)_2$ with Co^{2+}Oh sites. Electrochemical characterization reveals that α-$Co(OH)_2$ is more active than β-$Co(OH)_2$ towards OER. The better activity can be attributed to the presence of Co^{2+}Td sites in α-$Co(OH)_2$, which are more active than Co^{2+}Oh sites. Then, porous cobalt oxide nanoplates enriched with oxygen vacancies are synthesized based on α-$Co(OH)_2$. The large surface area of porous cobalt oxide nanoplates together with enriched oxygen vacancies provide more active sites, which promote faster exchange of intermediates and more efficient electron transfer. Finally, a novel self-templating strategy for the fabrication of composite CoO–MoO_2 nanocages with enhanced OER performance is proposed. By designing a nanocage structure and incorporating conductive MoO_2 to promote both mass and charge transfer, high OER activity as well as good stability in the resulting CoO–MoO_2 composite nanostructure can be achieved.

A02-36

Rh/Si, Os/Si and Ir/Si Nanocomposites as the Best Electrocatalysts designed for the Hydrogen Evolution Reaction

Xing Fan*, Haiping Lin, Youyong Li
Soochow University

The development of highly efficient electrocatalysts for HER (hydrogen evolution reation) is a fundamental undertaking of the hydrogen economy. We are committed to developing new HER catalysts with better catalytic activity, superior stability, and lower material cost than commercial Pt-based catalysts.

Herein, we investigated the electrocatalytic performance of M/Si (M = Os, Rh, Ir, Pt, Pd, Re, Ru, Au or Ag) nanocomposites for HER by experiments and theoretical DFT calculations.

The results indicated all the Rh/Si, Rh-Au/Si, Rh-Ag/Si, Os/Si and Ir/Si nanocomposites exhibit excellent HER catalytic efficiencies much better than commercial Pt-based catalysts even under industrial conditions (when the exchange current density is 1000mȦcm-2), especially for the Os/Si and Ir/Si nanocomposites.

The theoretical results revealed that such outstanding catalytic activity agree with that of experiment of the Os/Si ($\Delta GH^* = -0.03$ eV) and Ir/Si ($\Delta GH^* = 0.014$ eV) catalysts arises from the thermodynamically more favorable hydrogen adsorption free energy at the Os/Si and Ir/Si interfaces than that on platinum ($\Delta GH^* = -0.09$ eV), which owing to dividing the H2 generation process to three steps occurring on two different catalysts: H adsorption on metal atoms, H diffusion to silicon and H2 desorption from silicon.

A02-37

Interfacial Synthesis of Highly Stable CsPbX3/Oxide Janus Nanoparticles

Huicheng Hu*[1],Linzhong Wu[1],Yeshu Tan[1],Qixuan Zhong[1],Min Chen[1],Yinghua Qiu[1],Di Yang[1],Baoquan Sun[1],Qiao Zhang[1],Yadong Yin[2]
1. Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University
2. Department of Chemistry, University of California, Riverside

The poor stability of $CsPbX_3$ (X = Cl, Br, I) nanocrystals (NCs) has severely impeded their practical applications. Although there are some successful examples on encapsulating multiple $CsPbX_3$ NCs into an oxide or polymer matrix, it has remained a serious challenge for the surface modification/encapsulation using oxides or polymers at a single particle level. In this work, monodisperse $CsPbX_3/SiO_2$ and $CsPbBr_3/Ta_2O_5$ Janus nanoparticles were successfully prepared by combining a water-triggered transformation process and a sol−gel method. The $CsPbBr_3/SiO_2$ NCs exhibited a photoluminescence quantum yield of 80% and a lifetime of 19.8 ns. The product showed dramatically improved stability against destruction by air, water, and light irradiation. Upon continuous irradiation by intense UV light for 10 h, a film of the $CsPbBr_3/SiO_2$ Janus NCs showed only a slight drop (2%) in the PL intensity, while a control sample of unmodified $CsPbBr_3$ NCs displayed a 35% drop. We further highlighted the advantageous features of the $CsPbBr_3/SiO_2$ NCs in practical applications by using them as the green light source for the fabrication of a prototype white light emitting diode, and demonstrated a wide color gamut covering up to 138% of the National Television System Committee standard. This work not only provides a novel approach for the surface modification of individual $CsPbX_3$ NCs but also helps to address the challenging stability issue; therefore, it has an important implication toward their practical applications.

A02-38

Fabrication of Metal Sulfides with Hierarchical Micro/Nano-Structures and Their Applications in Energy Devices

Meidan Ye*, Xiaodan Hong, Qun Liu, Chunfeng He, Xiaoyue Gao
Xiamen University

Metal sulfides have attracted much attention because of their special photo/electric/manganic properties and great potential applications in catalysis, solar cells and energy storage.1-6 For example, metal sulfides could act as effective counter electrode alternatives to novel metal Pt and Au in quantum dot-sensitized solar cells due to their excellent electrocatalytic activity and stability in polysulfide electrolyte. Many experiments reveal that the chemical composition, crystal structures and micro-scale features all play important roles in their performance of metals sulfides. In this regard, the design and fabrication of metal sulfides with complicated micro/nano-structures will be very promising to enhance their performance in the energy conversion and storage devices. We have rationally prepared a series of metal sulfides (e.g., Cu_2S, $Cu_2Mo_6S_8$, $NiCo_2S_4$, $Co_9S_8/NiCo_2S_4$, etc.) via different chemical/physical routes. These metal sulfides showed attractive hierarchical features and excellent electrochemical properties when applied in solar cells, photocatalysis and energy storage devices.

A02-39

Thin film fabrication in perovskite solar cells

Qi Chen*
Beijing Institute of Technology

Perovskite photovoltaic is emerging as one of the most competitive solar technology due to its excellent optoelectronic property, such as high absorption coefficient, long carrier diffusion length. In view of recent advances in perovskite solar cell research, hysteresis, stability and PCE are the three most attracting topics among the community. The high power conversion efficiency (PCE) requires delicate control over the perovskite film and the relevant interfaces, and deep understanding of defects. This talk covers recent progress in our group regarding defects elimination, surface passivation and controllable facet orientation, which improves both efficiency and lifetime of perovskite solar cells. In addition, the fabrication cost is discussed, which determines the future commercialization path of this PV technology.

A02-40

Photocatalytic hydrogenation of carbon dioxide with high selectivity to methanol at atmospheric pressure

Le He
Soochow University

The production of solar methanol, directly from gaseous CO_2 and H_2, is important for the development of a sustainable energy economy. Despite growing activity in the field, very few photocatalysts exist that can efficiently and stably hydrogenate gaseous CO_2 to methanol at ambient pressure with high selectivity. Herein, we report that a defect laden indium oxide, $In_2O_{3-x}(OH)_y$, with a rod-like nanocrystal superstructure, can photocatalyze the hydrogenation of CO_2 to methanol with 50% selectivity under simulated solar irradiation. Notably, the solar methanol production of the $In_2O_{3-x}(OH)_y$ nanocrystal superstructures can be stabilized at a rate of 0.06 mmol $gcat^{-1}h^{-1}$ at atmospheric pressure. This is 120 times higher than that of the best-known photocatalysts. This discovery bodes well for the development of a low-pressure solar methanol process using CO_2 and renewable H_2 feedstocks.

A02-41

Antipulverization Anodes by Stress-relieved Structure Design for Robust Lithium Storage

Lianhai Zu, Ting He, Bingjie Cheng and Jinhu Yang*
School of Chemical Science and Engineering, Tongji University, Siping Road 1239, Shanghai 200092, P. R. China
Email: yangjinhu@tongji.edu.cn

As one of the current major energy storage technologies, lithium-ion batteries (LIBs) are widely expected to power emerging portable electronics and electric vehicles (EVs) [1,2]. To meet this demand, it is necessary to develop high-performance LIBs with long cycling stability. However, LIBs have long suffered from the severe pulverization of anode materials induced by huge volume changes upon Li-ion insertion/extraction, which causes irreversible capacity loss as well as poor cycling stability and rate capability [3,4]. To resolve the problem, it is necessary to explore antipulverization anode materials that can withstand severe lithiation and delithiation reactions for stable and robust lithium storage.

To this end, we propose the construction of novel mechanically stable structures and investigation of their unique stress-relieved properties as antipulverization LIB anodes. For example, we constructed a series of nanostructures/architectures such as SnO_2 triple-shelled hollow superstructures [5], Si-substituted $Zn_2(GeO_4)_{0.8}(SiO_4)_{0.2}$ nanowires [4] and mesoporous TiO_2/TiC@C composite membranes [6] and investigated their battery performance as well as antipulverzation mechanisms. It was found these anodes with such struture designs could realize antipulverizition upon lithiation/delithiation due to stress-relieved mechanisms in bulk phase or at interfaces of electrode materials at atomic- and nano-scale dimensions. The stress-relieved mechanisms involved were well studied and evidenced by substantial characterizations including mechanics simulations, in situ transmission electron microscopy and X-ray absorption fine structure spectroscopy. These studies open a new avenue in the development of antipulverization LIBs high-performance for practical energy applications.

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A02-42

Facet-Dependent Performance of Palladium-Catalyzed Selective Hydrogenation of Light Alkynes to olefins

Yong Xu*, Qiao Zhang
Soochow University

In comparison with polyethylene, polypropylene exhibit better resistance to acids, organic solvents, cracking, fatigues, and has therefore been used extensively in the automotive industry and the packaging industry. In the production process of polypropylene, however, the selective semi-hydrogenation of trace amounts of propyne to propene is a key step, because the presence of alkynes will poison the downstream catalysts used for polymerizations. Although the Pd based materials have been extensively investigated and reported as active and selective hydrogenation catalysts, the in-depth insights of their selective origins are far from available. Herein, combining theoretical calculations and experimental analysis, we show that the facet structure and catalytic selectivity is closely interrelated. The close packed {111} facets of Pd gives great propene selectivity (exceeding 95%) at low temperatures (30oC ~ 35oC) and atmospheric pressure. By contrast, the more open {100} facet tends to catalyze the full hydrogenation and thus give rise to poor propene selectivity of about 50%. By examining the DOS plots for the Pd surfaces with and without hydrogen atoms, we show that underlying mechanism of such facet-dependent selectivity can be interpreted by the shift of d-band center and hybriziation.Our experimental and computational results may provide strategically important information for improving catalytic performance in selective semi-hydrogenation of propyne to propene in large-scale industrial processes.

A02-43

Quantum dots Luminescent Solar Concentrators: From Concept to Real Application

Hongbo Li*
Beijing Institute of Technology

Luminescent solar concentrators (LSCs) are envisioned to reduce the cost of solar electricity by decreasing the usage of more expensive photovoltaic (PV) materials. Due to their high stability, high emission efficiencies and tuneable emission/absorption spectra, colloidal quantum dots (QDs) have emerged as very promising fluorophores for LSCs. An important advantage of the QDs over dye-based system is a possibility to greatly reduce re-absorption by independently adjusting the emission band and the onset of absorption, via the approaches commonly called as "Stokes-shift engineering." This presentation will discuss several approaches to Stokes-shift engineering with II-VI and I-III-VI QDs [1]. We will describe the first example of large area (up to ca. 90×30 cm^2) LSC based on specially engineered QDs, using standard doctor-blade deposition onto commercial window glasses [2]. Furthermore, we will give additional example of a large-area (>200 cm^2) tandem LSC based on two types of nearly reabsorption-free QDs spectrally-tuned for optimal solar-spectrum splitting [3]. Due to their strong performance achievable with low-cost, solution-processible materials, QD-based LSCs can provide a viable pathway for greatly reducing the cost of solar electricity by complementing the existing PV technology with inexpensive, high-efficiency sunlight collectors deployable either as strongly absorbing LSC-PV modules or semi-transparent building-integrated solar windows.

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A02-44

$g\text{-}C_3N_4$ embedded carbon dots for visible light photocatalytic H2 production

Zaicheng Sun*
Beijing University of Technology

Photocatalytic water splitting is considered as one of the promising ways to provide clean fuels. Extensive efforts have been made in the past to develop various inorganic and organic materials systems as photocatalysts for water splitting by using visible light. Among these photocatalysts, it was recently demonstrated that incorporation of carbon dots (CDs) into graphitic carbon nitride ($g\text{-}C_3N_4$) results in new metal-free composites (g- C_3N_4-C) with excellent stability and impressive performance for photocatalytic water splitting. However, fundamental questions still remain to be addressed such as how added CDs influence the photocatalytic reaction through the bandgap tunability, charge transfer route, and efficiency, as well as the specific function of CDs in the photocatalytic process. Understanding the chemical and physical behaviors of added CDs for the control of g- C_3N_4-C architecture is a critical need for its emergence from fundamental design of more efficient photocatalysts to practical applications. In this article, we report new materials with well-controlled architecture allowing for fine-tuning band gaps for broader visible light absorption and controlled understanding of the photocatalytic process. The well-defined model materials allow us to address the fundamental question regarding chemically bonding of CDs and how the chemical bonded CDs promote charge separation and transfer for highly efficient generation of H_2.

Keywords: $g\text{-}C_3N_4$, H_2 production, Photocatalytic

A02-45

CdS Nanoribbon-Based Memory Photodetectors

Zhibin Shao*, Tianhao Jiang, Jiansheng Jie
SooChow University

Ultraweak light detectors have applications in fields such as astronomical observation, remote sensing, laser ranging, and night vision. Nevertheless, the current commercial ultraweak light detectors based on a photomultiplier tube or an avalanche photodiode are not compatible with microelectronic devices in digital imaging applications due to their high operating voltage and bulky size.[1] Here we show a new class of memory photodetector (MPD) based on charge-storage accumulative effect at CdS nanoribbon (NR) surface, which exhibits an exponential-growth photoelectric conversion law. MPD breaks the cubic-growth photoelectric conversion law of the traditional photodetectors, and greatly improve the capability to detect ultraweak light. The suppression toward the dark current by the surface electric field, combined with long-term accumulation of photogenerated charges, enables MPD an unprecedentedly high responsivity of 3.8×10^9 A W^{-1} and detectivity of 7.7×10^{22} cm $Hz^{1/2}$ W^{-1}, which are 3-5 orders of magnitude higher than that of previously reported low-dimensional nanostructures-based photodetectors. As a result, the MPD devices can detect an ultraweak light at 6 nW cm^{-2} with an extremely high sensitivity of 4×10^7. In addition, delayed or real-time reading of light-triggered electrical output signals is successfully demonstrated. The proposed CdS NR based MPD device provides an insight into the design of the next generation of high performance and multifunctional integrated optoelectronic devices.

A02-46

pH Values Effects on Morphosynthesis of CaTi2O5 via a Facile Additive-Free Aqueous Strategy and its properties

Weixia Dong*, Qifu Bao
Department of material Science and Engineering, Jingdezhen Ceramic Institute, Jingdezhen, 333001, P. R. China

$CaTi_2O_5$ shuttle-like nanostructure have been selectively prepared by a solvothermal process without template and surfactant. The phase of the as-prepared samples was determined by X-ray diffraction (XRD). The microstructure were characterized by scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). Results found that pH values had a crucial effect on the crystal phase and shape evolution of the samples. $CaTi_2O_5$ sample prepared at pH of 5.2 shows high efficient light harvesting, large surface area and crystallinity. Moreover, $CaTi_2O_5$ shuttle-like sample shows good photocatalytic activity against methl orange due to its longer and thinner shuttle-like morphology and high crystallinity, enhanced light harvesting and large surface area. The photocatalytic rate (K) of $CaTi_2O_5$ shuttle-like structure reaches 0.1988 min^{-1} in 25 min for methyl orange (MO) degradation under the ultraviolet light irradiation and displays an excellent photostability with a degradation efficiency of 0.1952 min^{-1} after 4 cycles. And after combination with C_3N_4, $CaTi_2O_5$ showed an interesting catalytic behavior and the phtocatalytic activity of 99.6 % under visible light at 100 min.

A02-47

Cs_4PbX_6 (X = Cl, Br, I) Nanocrystals: Preparation, Water-Triggered Transformation Behavior, and Anti-Counterfeiting Application

Xiaoya Yu*, Qiao Zhang
Institute of Functional Nano and Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials and Devices, Soochow University, 199 Ren'ai Road, Suzhou, 215123, Jiangsu, People's Republic of China.

As a promising material, Cs_4PbX_6 (X = Cl, Br, I) nanocrystals (NCs) have attracted much attention. However, their luminescent property is still under debate. In this work, we first systematically studied the colloidal preparation of Cs_4PbX_6 NCs. It is found that the critical parameter for the formation of Cs_4PbX_6 NCs is the ratio between Cs and Pb. Pure Cs_4PbX_6 NCs are non-luminescent. The luminescence property of previous reported Cs_4PbX_6 NCs may come from the impurity of luminescent $CsPbX_3$ NCs. No co-existence of both Cs_4PbX_6 and $CsPbX_3$ phases has been found in one single nanoparticle. The water-triggered transformation from nonluminescent Cs_4PbX_6 NCs to luminescent $CsPbX_3$ NCs has been quantitatively studied. The potential application of Cs_4PbX_6 NCs in humidity sensor and anti-counterfeiting have been demonstrated. This work is important because it not only confirmed the non-luminescent nature of Cs_4PbX_6 NCs but also demonstrated the potential application of such NCs.

A02-48

A Core–Shell System Based on Binary Transition Metal Sulfide Toward Synergetic Electrocatalytic Water Splitting

Han Zhu*, Songge Zhang, Chen Liu, Mingliang Du
Jiangnan University

The production of hydrogen and oxygen through water splitting are promising and appealing solution for developing clean-energy technologies. To optimize and enhance electrocatalysts performance and durability for the hydrogen and oxygen evolution reactions through electrolysis, we describe a new class of $Co_9S_8@MoS_2$ core-shell structures formed on carbon nanofibers with cubic Co_9S_8 as cores and layered layered MoS_2 as shells. The core-shell design of these nanostructures allows us to combine the advantages of MoS_2 and Co_9S_8, serving as switchable electrocatalyst for H_2 and O_2 evolutions. The unique $Co_9S_8@MoS_2$ demonstrates low onset potentials and overpotentials at j=10 mA/cm^2 of 64 and 190 mV for HER and 350 and 430 mV for OER, respectively, when compared with individual MoS_2 and Co_9S_8 phase. The high hydrogen and oxygen evolution activities of the $Co_9S_8@MoS_2$ is due to the electrocatalytic synergetic effects of nano-interfaces generated by directly contact regions between the Co_9S_8 and MoS_2 shell. These advantages can generate strong electron transfer between Co and Mo through the intermediate sulfur atoms bonded to both metals, leading to the promising promoted electrocatalytic activity.

A02-49

Crystal Surface Control of Photocatalysts Exhibiting Enhanced Photocatalytic Performance

Ping Li
Institute of Advanced Material, Nanjing Tech University, 5 Xin Mo Fan Road, Nanjing, 210009

Supplying the word with sustainable energy is one of the most pressing issues in modern society. Micro/nanostructures with carefully controlled crystal surface can be applied to photocatalytic applications. In this report, I will present two examples of crystal facets exposed semiconductor for solar energy conversion.

We report an unprecedented, crystal facet-based CeO2 homojunction consisting of hexahedron prismanchored octahedron with exposed prism surface of {100} facets and octahedron surface of {111} facets which was fabricated through solution-based crystallographic-oriented epitaxial growth. We expended high-index crystal facets to ternary inorganic compound. Unprecedented 30-faceted BiVO4 polyhedra predominantly surrounded by {132}, {321}, and {121} high-index facets are fabricated through the engineering of high-index surfaces by a trace amount of Au nanoparticles.

A02-50

Nanostructured Transition Metal Nitrides for Advanced Electrochemical Energy Storage

Kaifu Huo*
Huazhong University of Science and Technology

With increasing demands of portable electronic products, renewable energy, and hybrid electrical vehicles, high performance energy storage devices have attracted worldwide attention. Rechargeable lithium-ion battery and supercapacitors (SCs) are the most promising electrochemical energy storage devices in terms of energy density and power density, respectively. The electrode material is the key component of an energy storage device, determining the capacitive properties of the device. Transition metal nitrides (TMNs) such as VN, TiN and Mo_2N nanostructures have gained enormous interest as electrode materials for next-generation high performance SCs and batteries owing to their excellent electrical conductivity, high specific capacitance and low-cost. In this talk, we will introduce our recent progress on nanostructured metal nitride electrode materials for high-performance flexible SCs, Li-S batteries and electrochemical hydrogen generation. The high-performance electrodes based on TMNs exhibit excellent capacitive properties and robust mechanical integrity for flexible SCs, excellent electrochemical catalytic activity (HER and OER) and superior Li-S battery performance, enabling their promising applications in high-performance energy storage devices.

A02-51

Metal Halide Nanomaterials: the Synthesis and optoelectronic devices

Hongbin Yao*, Kun-Hua Wang, Ji-Song Yao
University of Science and Technology of China

Metal halide perovskite nanocrystals emerged as an attractive semiconducting nanomaterials due to their excellent properties such as well-defined nanostructures, tunable band gaps, high carrier mobilities, low non-radiative recombination, and low cost. The optoelectronic detectors and light-emitting diodes based on the metal halide perovskite nanocrystals have the potentials to gain high efficiencies owing to the facilitated separation-combination of carriers in the confined nanocrystals. Here, we reported a series of perovskite nanocrystals and their facile synthesis, assemblies and ion-dopings for optoelectronic devices. We developed antisolvent precipitation method to synthesize highly luminescent $CsPb_2Br_5$ nanosheets and investigated their anion exchange to tune the bandgaps. In addition, we used ion-doping strategy to modulate the photoluminescent kinetics in $CsPbBr_3$ nanocrystals and the resulted external quantum efficiency of as-fabricated light emitting diode increased around ~4 folds. Finally, we explored a new kind of photoluminescent nanomaterials based on the lead-free copper iodide-ligand hybrid clusters and its application as photoluminescent ink for painting and solid light emitting coating.

A02-52

All-solid-state flexible micro-supercapacitor for wireless monitoring system

Weiqing Yang*, Haichao Huang, Haitao Zhang, Hai Su, Xiang Chu
South west Jiaotong University

As an integrated signal monitoring and transmission device which is real-time, uninterrupted and require no external energy supply, self-powered wireless monitoring systems has significant value of application in various signal monitoring fields, such as dynamic monitoring of the operating status of high-speed trains and aeroengines. For this systems, supercapacitors hold an important status in energy storage. Due to high power density, fast charge and discharge capabilities, and excellent cycle stability, supercapacitors play an important role in energy storage in wireless security monitoring systems. Among them, all-solid-state flexible supercapacitors occupy an important position with their excellent flexibility and portability.

In order to obtain flexible micro-supercapacitors with excellent electrochemical performance, we have achieved the growth of hierarchical tubular carbon nanotubes (hCTNs) on flexible stainless steel meshes based on magnesium thermal deposition reactions. And the assembled flexible supercapacitor exhibits a high area capacitance of ~320 mF cm^{-2}, as well as good rate performance and excellent cycling stability. Secondly, the Ti_3AlC_2 MAX phase ceramic was selective etched by HCl+LiF to obtain the two dimensional $Ti_3C_2T_x$ (MXene). In combination with vacuum filtration and micro-fabrication techniques, the free-standing MXene films was obtained with excellent flexibility. The all-solid-state flexible supercapacitor based on free-standing MXene films exhibits high areal capacitance up to 340 mF cm^{-2} and ultrahigh volumetric capacitance of 183 F cm^{-3} at 0.25 mA cm^{-2}. In addition, we fabricated MXene based paper supercapacitor which shows area capacitance of ~64 mF cm^{-2}, excellent flexibility and cycle stability. Finally, we used electrochemical polymerization method to prepare three-dimensional network polyaniline/phytic acid hydrogels cross-linked in situ on flexible PET film. Polyaniline/phytic acid based interdigitated flexible supercapacitors exhibit good flexibility and can maintain stable electrochemical performance under bending, twisting, and other stress conditions. The surface capacitance can reach 136.0 mF cm^{-2} at a current density of 1 mA cm^{-2}.

The all-solid-state flexible supercapacitors based on hierarchical tubular carbon nanotubes, MXene, and polyaniline/phytic acid all exhibit excellent electrochemical performance, demonstrating the potential applications of these materials in wireless monitoring system.

A02-53

Controlled preparation of $ZnCo_2O_4$ nanostructures for asymmetric supercapacitor with ultrahigh energy density

Yan Zhao*
Jiangsu University

Porous $ZnCo_2O_4$ nanostructures with hexamethylenetetramine (HMT) as adscititious alkali are fabricated via a facile hydrothermal route and heat treatment process. The morphology of the materials can be easily tuned from nanowires to nanobelts by simple varying the hydrothermal temperature. Due to the superiority of the porous nanostructure and the convenient ion transport, the obtained $ZnCo_2O_4$ nanostructures are further applied as electrode materials for supercapacitors and exhibit noticeable pseudocapacitive performance with high specific capacitance of 776.2 F g^{-1} at 1 A g^{-1} and good cycle stability (84.3% capacity retention at 3 A g^{-1}). Moreover, a high-voltage asymmetric supercapacitor using the $ZnCo_2O_4$ as the anode assembled with the freeze-dried reduced graphene oxide (F-RGO) cathode displays superior electrochemical performance with an ultrahigh energy density (84.48 Wh kg^{-1} at 0.4 kW kg^{-1}), which reveals a great promise for practical application in electrochemical devices.

A02-54

Chlorination of the π-conjugated polymer: A facile way for efficient solar energy conversion

Feng He*
Southern University of Science and Technology

With the development of material engineering, interface modification, and advanced device processing in past decades, the power conversion efficiency (PCE) of the state-of-the-art PSCs has already exceeded 13% at present. Especially, the benzothidiazole-T4 families of polymers, such as PffBT4T-2OD, have attracted tremendous research interest in academic communities since they can be processed into highly efficient fullerene/polymer solar cells with power conversions up to 10%. Herein, we designed and synthesized a chlorinated polymer donor, PBT_4T-Cl, in which a chorine atom had been introduced at the middle thiophene unit to fine tune the energy level of the final polymers. Compared with its non-chlorinated analog, the PBT_4T-Cl-based devices exhibited clear increases in open-circuit voltage and fill factor, achieving PCEs up to 11.18%, which is the highest PCE of a chlorine-based PSC reported to date. GIWAXS analysis illustrated the strong crystallinity from the blend films, AFM and TEM measurements both revealed an optimized morphology of the spin-coated PBT_4T-Cl blend films, all of which supported that chlorine substitution could promote the performance of PSCs. More importantly, the PBT_4T-Cl-based devices showed superior stability, with a PCE of 8.16% after 50 days device storage, while the non-Cl-analog-based devices remained at only 5.36% in a parallel experiment. Through this research, the chlorination of low band gap polymers provides new insight into designing π-conjugated polymer semiconductors and realizing further enhancement of polymer solar cell efficiency as well as stability.

A02-55

Ultrasmall/Ultrathin Noble Metal Nanomaterials for Energy-Related Catalytic Reactions

Chuanbo Gao*
Xi'an Jiaotong University

Objective: Ultrasmall or ultrathin (angstroms to a few nanometers) noble metal nanomaterials promise excellent activity in many energy-related catalytic reactions due to the high ratio of surface atoms and size-dependent electronic properties. Both the precise size engineering and the understanding of the correlation between the size of noble metal nanoparticles and their catalytic properties remain far from complete. In this work, we aim to synthesize noble metal nanomaterials (zero-dimensional nanoparticles, one-dimensional nanowires, and two-dimensional nanoplates or nanoribbons) with precise control, and reveal their enhanced catalytic properties.

Methods and Results: Ultrasmall nanoparticles of noble metals, Pt for example, were successfully synthesized in reverse micelles, which have been further encapsulated in hollow titania nanospheres by the in situ titania coating and subsequent annealing. The Pt@TiO2 yolk/shell nanospheres display extraordinary stability and size-dependent activity in the water-gas shift (WGS) reaction, making them potentially applicable in mobile hydrogen fuel cell systems. The size-dependent variation in the electronic property of the Pt nanoparticles and the reducible oxide encapsulation that prevents the Pt nanoparticles from sintering are ascribed as main reasons for the excellent catalytic performance.

In addition, strategies have been developed for the synthesis of ultrathin Pt-alloy nanowires, nanoplates, and nanoribbons in a simple, efficient, and cost-effective manner. Specifically, these nanomaterials were prepared by a templating strategy and a hydrothermal method, which demonstrate superior activities in the hydrogen evolution reaction (HER), methanol oxidation reaction (MOR), and oxygen reduction reaction (ORR), respectively, and thus hold a promise in water-alkali or chlor-alkali electrolyzer and direct-methanol fuel cell applications.

Conclusions: In summary, we demonstrate robust strategies to synthesize a diversity of noble metal nanomaterials with ultrasmall, precisely-controlled sizes, and reveal their enhanced catalytic activities. The high surface area and size-dependent property of the noble metal nanomaterials are found to be responsible for the enhanced catalytic performance. We believe these findings open new opportunities in the catalyst design for a broad range of energy-related catalytic reactions.

A02-56

Piezo-electret Gated MoS2 Field Effect Transistor for Sensory Application

Jing Zhao*[1], Guangyu Zhang[2], Qijun Sun[1], Zhonglin Wang[1]
1. Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences
2. Institute of Physics, Chinese Academy of Sciences

Molybdenum disulfide, one of typical two-dimensional materials, draw more attention due to its fantastic electrical property for as field effect transistors (FETs). However, the traditional FETs based on chemical vapor deposited monolayer MoS2, controlled by an externally supplied gate voltage, is not sensitive enough to respond to applied strain. Here, we reported a novel MoS2 FET gated by ferro-/piezo-electrets for potential sensory applications. Ferro-/Piezo-electrets (poly(vinylidene fluoride-trifluoroethylene)) can be used as transducer materials due to not only their longitudinal piezoelectricity but also their maintainable potentials after initial polarization. Therefore, the transport property of MoS2 FET can be sensitively tunable by the electret film while the small strain varying from -0.4% to 0.2%. In addition, both stable and reproduceable static and dynamic regulation can be realized, which provides broad application prospects for artificial electrical skin.

A02-57

Polymer electrolyte based All-solid-supercapacitors: flexibility, self-healing and integration with functional devices

Jian Yan[1], Yan Jian[2], Wu Yucheng[2]
1. Hefei University of Technology
2. Schcool of Materials and Engineering, Hefei University of Technology, Hefei 230009, China.

Polybenzimidazole (PBI) when doped with acid or alkaline is one kind of solid polymer electrolytes, which exhibits much higher mechanical strength over gel-electrolytes. It is suitable for the all-solid-supercapacitors. We report two kinds of PBI based all-solid-supercapacitors. One is the flexible supercapcitor with specific capacitance well maintained under deformation of bending, twisting, winding and repeated bending. Such devices also show high mechanical strength with tensile strength up to ~100 MPa. The ESR value of devices is similar to that of gel-electrolytes based devices.[1,2] Asymmetric foldable devices using AC/CNT-Ni$(OH)_2$ or AC/Ni-Co MOF design exhibit a high specific capacitance up to 160 F/g within 1.5V window.[3] The other one is the self-healing supercapacitor. By mixing self-healing polymer as binder, polyaniline (or composites), PBI and Super-P the electrode, self-healable symmetric all-solid-supercapacitors have be fabricated. This kind of self-healable supercapacitors exhibits very good cycling stability. The capacitance retention is above 90%

after 10000 cycles which is significantly improved compared to that of pure PANI electrode. Such enhancement is due to the self-healing behavior and all-soild design since the mechanical damage caused by volume change of PANI based electrodes. This kind of all-solid-supercapacitor could also be integrated with generator to become multi-functional devices.

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A02-58

Rod-like anatase TiO2 mesocrystals composited with Au nanoparticles in controlled locations for enhanced photocatalytic activity

Xiaxi Yao*, Wenjun Zhang, Xiuli Hu, Xuhong Wang
Changshu Institute of Technology

Anatase TiO_2 nanocrystals with [001] orientation have attracted great attention due to the fast spatial charge separation, while anatase TiO_2 mesocrystals become the research topic because of the high crystallinity and large surface area. In this work, rod-like anatase TiO_2 mesocrystals along [001] direction were successfully synthesized by a one-step solvothermal method with tetraethyl silicate (TEOS) as the stabilizer and barium acetate as the additive. The as-prepared anatase TiO_2 mesocrystals were composed of small nanocrystals with size of 9 nm and showed the uniform rod-like morphology. The exposed (101) surface of TiO_2 mesocrystals provided numbers of active reduction sites and were favorable for the loading of Au nanoparticles under photocatalytic conditions. The Au-TiO_2 mesocrystals showed high photocatalytic activity in the photodegradation of organic dyes and excellent photocatalytic H_2-evolution performance from water splitting. A feasible mechanism was proposed for the photogenerated electrons transfer in the composite system.

A02-59

From Nonluminescent Cs4PbX6 (X = Cl, Br, I) Nanocrystals to Highly Luminescent CsPbX3 Nanocrystals: Water-Triggered Transformation through a CsX-Stripping Mechanism

Linzhong Wu*, Qiao Zhang
Institute of Functional Nano & Soft Materials, Soochow University

We report a novel CsX-stripping mechanism that enables the efficient chemical transformation of nonluminescent Cs_4PbX_6 (X = Cl, Br, I) nanocrystals (NCs) to highly luminescent $CsPbX_3$ NCs. During the transformation, Cs_4PbX_6 NCs dispersed in a nonpolar solvent are converted into $CsPbX_3$ NCs by stripping CsX through an interfacial reaction with water in a different phase. This process takes advantage of the high solubility of CsX in water as well as the ionic nature and high ion diffusion property of Cs_4PbX_6 NCs, and produces monodisperse and air-stable $CsPbX_3$ NCs with controllable halide composition, tunable emission wavelength covering the full visible range, narrow emission width, and high photoluminescent quantum yield (up to 75%). An additional advantage is that this is a clean synthesis as Cs_4PbX_6 NCs are converted into $CsPbX_3$ NCs in the nonpolar phase while the byproduct of CsX is formed in water that could be easily separated from the organic phase. The as-prepared $CsPbX_3$ NCs show enhanced stability against moisture because of the passivated surface. Our finding not only provides a new pathway for the preparation of highly luminescent $CsPbX_3$ NCs but also adds insights into the chemical transformation behavior and stabilization mechanism of these emerging perovskite nanocrystals.

A02-60

Cd^{2+}-doped amorphous TiO_2 hollow spheres for robust and ultrasensitive photoelectrochemical sensing of hydrogen sulfide

Hongbo Li*[1,2], Jing Li[1], Yunyun Zhu[1], Wenyu Xie[1], Rong Shao[1], Xiaxi Yao[2], Aiqin Gao[2], Yadong Yin[2]
1. Yancheng Institute of Technology
2. University of California, Riverside

Hydrogen sulfide is a highly toxic molecule to human health, but its high-performance detection remains a challenge. Herein, we report an ultrasensitive photoelectrochemical (PEC) sensor for H_2S by modifying indium tin oxide (ITO) electrodes with Cd^{2+}-doped amorphous TiO_2 hollow spheres, which are prepared by templating against colloidal silica particles followed by a

cadmium-sodium cation exchange reaction. The amorphous TiO_2 hollow spheres act as both the probing cation carrier and the photoelectric beacon. Upon exposure to sulfide ions, the photocurrent of the functionalized photoanode proportionately decreases in response to the formation of CdS nanoparticles. This could be explained that the mismatching band gap between amorphous TiO_2 and CdS nanoparticles results in the part of photoexcited electrons and holes from amorphous TiO_2 transferred to the conduction band and valence band of CdS nanoparticles, respectively. And then the carriers recombined at CdS nanoparticles and caused the decreased photocurrent therefore. The decreasement of photocurrent is linear with the concentration of sulfide ions in the range from 1 to 10000 pmol L^{-1} with a detection limit of 0.36 pmol L^{-1}. Enabled by a unique sensitization mechanism, this PEC sensor features excellent performance in a wide linear range, high selectivity and sensitivity, high stability, and low fabrication cost.

A02-61

Mineral Nanomaterials Enable High-Efficiency Electrocatalysis

Minrui Gao*
University of Science and Technology of China

The development of pyrite-type catalysts provides new perspectives in the search for efficient and robust Earth-abundant catalysts[1,2]. These crystalline solids contain the characteristic dianion units and have cations occurring in octahedral coordination-whose generalized formula is MX_2, where M = Fe, Co or Ni and X is a chalcogen. The properties of metal pyrites are diverse, ranging from semiconductors such as FeS_2 to metals such as CoS_2 and $CoSe_2$. Moreover, pyrite-type structures can be extended to transition metal dichalcogenides consisting of ternary elements, for examples, CoAsS (cobaltite), NiAsS (gersdorfffite), NiSbS (ullmannite), CoPS and others, offering this family of materials rich chemistry, versatile and tunable properties. In recent years research on the synthesis of pyrite nanomaterials and on related structure understanding has dramatically advanced their applications. In this Symposium, we want to discuss recently demonstrated applications of nanostructured pyrite-type materials in the field of electrocatalysis [3-7]. We first briefly highlight some interesting properties of pyrite-type materials and why they are attractive for modern electrocatalysis. Some recent progress on their synthesis that allows the access to highly nanostructured pyrite-type materials is reviewed along with the coupling of resulting pyrites with other functional objects (e.g., metal oxides, metal chalcogenides, noble metals and carbons) to enable improved catalytic performances. We finally spotlight the exciting examples where pyrite nanostructures were used as efficient electrocatalysts to drive “water-hydrogen/oxygen” transformations.

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A02-62

Hydrogen Oxidation Reaction Electrocatalysts in Alkaline Electrolyte

Zhongbin Zhuang*
Beijing University of Chemical Technology

Fuel cell is clean and efficient energy conversion device that can directly convert chemical energy to electricity. Polymer electrolyte membrane fuel cells are promising due to their high power density and rapid start up capabilities. In particular, anion exchange membrane fuel cell (AEMFC) has gained much attention because of its potential for the use of non-precious metal based catalysts. However, on the anode side, where hydrogen oxidation reaction (HOR) occurs, it required much more Pt loading than the acidic proton exchange membrane fuel cell to get the same cell performance. Thus low cost, high performance hydrogen oxidation reaction (HOR) catalyst in alkaline condition is still challenging. Here, we studied the HOR mechanism in alkaline condition by using surface controlled PtNi nanoparticle model catalysts. We found that the HOR activity is mainly controlled by the hydrogen binding energy, while the influence of OH binding is not significant. We further developed nickel supported on nitrogen doped carbon nanotubes (Ni/N-CNT) as highly active non-precious metal based HOR catalyst in alkaline environment. The promoted catalytic activity is attribute to the synergistic effect of the support that makes nickel has optimized hydrogen binding energy.

Keywords: fule cell, hydrogen oxidation reaction, alkaline electrolyte, hydrogen binding energy

A02-63

Defect Engineering of Two-Dimensional Layered Materials

Ruitao Lv
Key Laboratory of Advanced Materials (MOE), School of Materials Science and Engineering, Tsinghua University

A02-64

Atomic configurations, electronic structures and catalysis: investigations from first principles calculations

Haiping Lin*.
Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University

The first-principles calculations have been widely employed for the analysis and interpretation of experimental observations. The first part of this presentation is to discuss our recent progress in the development of first-principles STM simulation methods and their applications in the field structural determinations and analysis of on-surface reaction mechanisms. Based on such structural information, theoretical studies can help to obtain the atomic insights of the catalytic origins, and thus provide important guidelines to the rational design of new catalysis. In the second part, I would like to present our recent researches in the design concept of a few heterogeneous catalysts, which exhibit outstanding water splitting catalytic activities, which surpass the corresponding commercial Pt/C for HER and RuO_2 for OER.

A02-65

Organic conjugated polymer for emerging perovskite solar cells

Jianyu Yuan*, Wanli Ma
Soochow University

In this contribution, a facile and universal method is successfully reported to fabricate perovskite solar cells (PSCs) with enhanced effciency and stability.Through dissolving functional conjugated polymers in antisolvent chlorobenzene to treat the spinning CH3NH3PbI3 perovskite flm, the resultant devices exhibit signifcantly enhanced effciency and longevity simultaneously. In-depth characterizations demonstrate that thin polymer layer well covers the top surface of perovskite flm, resulting in certain surface passivation and morphology modifcation. More importantly, it is shown that through rational chemical modifcation, namely molecular fuorination, the air stability and photostability of the perovskite solar cells are remarkably enhanced. Considering the vast selection of conjugated polymer materials and easy functional design, promising new results are expected in further enhancement of device performance. It is believed that the fndings provide exciting insights into the role of conjugated polymer in improving the current perovskite-based solar cells.

A02-66

Metal Charge Transfer Doped Carbon Dots with Reversibly Switchable, Ultra-High Quantum Yield Photoluminscence

Quan Xu*, Rigu Su
China University of Petroleum (Beijing)

As a class of the heteroatom-doped carbon materials, metal charge-transfer doped carbon dots (CDs) exhibited an excellent optical performance and were widely used as fluorescent probes. To improve fluorescence quantum yield (QY) remains one of the fundamental and challenging issues in the carbon dots field. Herein, we prepared a novel manganese doped CDs (Mn-CDs), which exhibited an ultra-high quantum yield of 54% - the highest quantum yield for metal-doped CDs. Various spectroscopic measurements revealed an in-situ change of dopant oxidation state during the synthesis. Our further study indicated the presence of metal-carbonate, which served as an important component for high quantum yield. We have also studied the reversibly switchable fluorescence property of Mn-CDs by adding Hg^{2+}/S^{2-}, as well as elucidating the underlying mechanism of this switching fluorescence

phenomenon. By using the Mn-CDs as fluorescent probes, we developed an extremely sensitive detection method for heavy metal Hg^{2+} detection at a nM detection limit level.

A02-67

Design and Engineering of Low-dimensional Transition-metal Chalcogenide Nanocrystals/Nanofibers and Their Electrocatalytic Applications

Mingliang Du*, Chen Liu, Han Zhu
Jiangnan University

Transition metal dichalcogenides (TMDs) have recently attracted substantial attention due to their potential application in the catalysis of the hydrogen evolution reaction (HER). In this study, triangular WSe_2 and $W(Se_xS_{1-x})_2$ nanoflakes uniformly dispersed on the surface of electrospun carbon nanofiber mats were synthesized in a chemical vapor deposition (CVD) system. The morphology and structure of these products were systematically characterized, revealing that WSe_2 nanoflakes are configured in the 2H phase with high crystallinity, and the $W(Se_xS_{1-x})_2$ nanoflakes are configured in the alloy form without any obvious phase separation. The hybrid catalyst mats were directly used as hydrogen evolution cathodes to investigate their HER activity. Excellent HER performances, including low overpotential, high current density and long-term stability, were achieved by optimizing the content of the initial W precursor and the appropriate substitution of selenium with sulfur, which resulted from the appropriate cover density and thickness of the WSe2 nanoflakes and the defective structure of the $W(Se_xS_{1-x})_2$ nanoflakes.

A02-68

Self-Assembled Porphyrin Nanocrystals for Efficient Visible-Light-Driven Hydrogen Evolution

Feng Bai*
Key Laboratory for Special Functional Materials of the Ministry of Education, Henan University

Molecular self-assembly is a powerful method to the synthesis of nanostructured materials with fine-tuning of the morphology and size. Through designing molecules and supramolecular entities, desired structure and function can be achieved. Porphyrin and its derivatives with macrocyclic aromatic conjugation system were excellent organic semiconductor materials and ideal building blocks based on the unique planar, rigid molecular geometry. With recent progress made during several years, we proposed an Emulsion-based assembly strategy to fabricate nanostructured porphyrin assemblies with programmed geometry and dimensions. By rational control of different combinations of porphyrins, surfactants and their concentration, hierarchical structured porphyrin nanocrystals (e.g. nanoparticles, Nanorods, nanowires and nanobelts) designed with short charge diffusion length, high crystallinity and less defects have been fabricated, which exhibit morphology and shape dependent photocatalytic hydrogen evolution activities. Molecular self-assembly plays pivotal roles in improving both the activity and reliability of porphyrin assemblies photocatalysts: (i) These assemblies exhibit collective and tailorable optical properties, thereby allowing broader and red-shift absorption spectrum, especially in the visible light region. (ii) Owing to the existence of surfactants, porphyrin assemblies can achieve the good dispersity in water. (iii) Ordered π−π stacks and long-range conjugated π-delocalization of porphyrin assemblies can reduce the migration distance of charge carriers, which mainly contributes to its remarkable photocatalytic properties. Overall, these findings present a new platform for the development of high-efficiency photocatalysts based on self-assembled supramolecular systems.

Keywords: photocatalytic hydrogen evolution, porphyrin, controllable self-assembly, visible-light

A02-69

Antipulverization Anodes by Stress-relieved Structure Design for Robust Lithium Storage

Lianhai Zu, Ting He, Bingjie Cheng and Jinhu Yang*
School of Chemical Science and Engineering, Tongji University, Siping Road 1239, Shanghai 200092, P. R. China
Email: yangjinhu@tongji.edu.cn

As one of the current major energy storage technologies, lithium-ion batteries (LIBs) are widely expected to power emerging portable electronics and electric vehicles (EVs) [1,2]. To meet this demand, it is necessary to develop high-performance LIBs with long cycling stability. However, LIBs have long suffered from the severe pulverization of anode materials induced by huge volume changes upon Li-ion insertion/extraction, which causes irreversible capacity loss as well as poor cycling stability and rate capability

[3,4]. To resolve the problem, it is necessary to explore antipulverization anode materials that can withstand severe lithiation and delithiation reactions for stable and robust lithium storage.

To this end, we propose the construction of novel mechanically stable structures and investigation of their unique stress-relieved properties as antipulverization LIB anodes. For example, we constructed a series of nanostructures/architectures such as SnO_2 triple-shelled hollow superstructures [5], Si-substituted $Zn_2(GeO_4)_{0.8}(SiO_4)_{0.2}$ nanowires [4] and mesoporous TiO_2/TiC@C composite membranes [6] and investigated their battery performance as well as antipulverzation mechanisms. It was found these anodes with such struture designs could realize antipulverizition upon lithiation/delithiation due to stress-relieved mechanisms in bulk phase or at interfaces of electrode materials at atomic- and nano-scale dimensions. The stress-relieved mechanisms involved were well studied and evidenced by substantial characterizations including mechanics simulations, in situ transmission electron microscopy and X-ray absorption fine structure spectroscopy. These studies open a new avenue in the development of antipulverization LIBs high-performance for practical energy applications.

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A02-70

Textile energy storage and harvesting devices as wearable power sources

Xiong Pu*
1.Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences
2.School of Nanoscience and Technology, Unersity of Chinese Academy of Sciences

Rapid advancements in wearable smart textiles and stretchable/multifunctional electronics impose the challenge on corresponding power devices that they should possess comparable flexibility, stretchability and functionalities. In this talk, we briefly summarize our recent progresses on wearable energy storage and harvesting devices, especially energy devices aiming to power smart textiles and artificial electronic skins. Both yarn or textile-based electrochemical energy storage devices and textile-based triboelectric nanogenerators (TENGs) have been developed; meantime, self-charging systems have been achieved by integrating them so that energies harvested from daily human motions can be stored simultaneously. It is even more challenging to provide power sources for electronic skins or soft electronics/robotics. We report a soft skin-like triboelectric nanogenerator that enables both biomechanical energy harvesting and tactile sensing by hybridizing elastomer and ionic hydrogel as the electrification layer and electrode, respectively. Ultra-high stretchability and transparency are achieved simultaneously for an energy-harvesting device. Lastly, we report our updated progresses on self-healable soft TENGs by utilizing self-healable elastomers. Buckled thin layers of conductive polymers are achieved by transfer the film onto pre-strained self-healable elastomers, which later ensure the realization of self-healing, stretchability, and transparency of the TENG simultaneously. Our work provides new opportunities for soft power sources and potential applications in soft/wearable electronics.

Keywords: Textile, energy storage, energy harvesting, wearable

A02-71

Explorations of Electrocatalysts for Application in High Energy Density Lithium- or Zinc-air Batteries

Chaohe Xu*, Xiaolong Guo
Chongqing University

Rechargeable metal-air batteries are receiving intensive interest due to their high theoretical specific energy, which far exceeds that of traditional batteries. However, current metal-air batteries suffered from serious problems, such as poor cycle life and low round trip efficiency, which obstacle their widely applications. Therefore, rational designs of highly active electrocatalysts are extremely important for improving the electrochemical performances of future metal-air batteries.

Herein, we first designed a two-step preparation of a highly active oxygen electrocatalyst based on ultra-small cobalt nanoparticles stabilized in a nitrogen-doped graphene matrix. The catalyst performs as well as the commercial Pt/C catalyst in the oxygen reduction reaction, and better than the Pt/C catalyst in the oxygen evolution reaction. This particular electrocatalyst could significantly lower the overpotential of oxygen electrochemical reactions in aqueous lithium-air batteries to attain a round-trip efficiency of about 79.0% at a current density of 0.1 mA cm^{-2}, thereby surpassing the performance of commercial Pt/C catalyst. We also developed a $NiCo_2O_4$@NiMn LDHs core-shell structure on nickel foam by hydrothermal reaction for using as electrocatalysts of Zn-air battery. The overpotential was only 254 mV at current density of 10 mA cm^{-2}, much lower than pure $NiCo_2O_4$ nanowires (334 mV) or LDHs nanosheets (279 mV); and the Tafel slope was as low as 67.3 mV dec^{-1}, which could be attributed to the higher electrochemical surface area of the core-shell structure. In long term stability characterization, there was only 6% increase during a 20 hours continuous operation. By employing it as air breathing electrode, the assembled Zn-air batteries could deliver more than 350 continues cycles with almost no apparent overpotential increases. Our results significantly highlighted that the rational designs of electrocatalysts are much important for further improving the electrochemical performances of future metal-air batteries.

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Keywords: Metal-air batteries, graphene, layered double hydroxide, electrocatalysts, oxygen reduction reaction

A02-72

Highly-efficient Nanocatalysts for the Chemical Transformation of CO and CO_2

Liangbing Wang*
Central South University

Hydrogenation of CO_2 into fuels and useful chemicals helps mitigate energy crisis by reducing the reliance on fossil fuels. The chemical transformation of CO_2 has been industrially achieved over heterogeneous $Cu/ZnO/Al_2O_3$ catalysts, which requires rigorous reaction conditions such as high pressure (50-100 bar) and elevated temperature (200-300 ^oC) because of the chemical inertness of CO_2. During the past decades, a vast variety of strategies have been developed to boost the catalytic activity toward CO_2 hydrogenation. Although the past decades have witnessed the great progress in improving the catalytic activity for CO_2 hydrogenation, it is still desiderated to develop highly efficient catalysts, especially for non-noble metal catalysts. Herein, we demonstrated a simple and effective strategy to modify non-noble metal catalysts by incorporating N atoms into Co nanosheets to boost the catalytic activity toward CO_2 hydrogenation. In CO_2 hydrogenation, Co_4N nanosheets exhibited turnover frequency number of 25.6 h^{-1} under 32 bar at 150 ^oC, which was 64 times as high as that of Co nanosheets. The activation energy for Co_4N nanosheets was 43.3 kJ mol^{-1}, less than half of that for Co nanosheets. Further mechanistic studies revealed that Co_4NH_x was formed by adsorbing H atoms on N atoms in Co_4N nanosheets in the presence of H_2. The amido-hydrogen atoms in Co_4NH_x directly added to CO_2 to form HCOO* as the intermediates. In addition, the adsorbed H_2O* was found to activate the amido-hydrogen atoms via the interaction of hydrogen bonds, facilitating the hydrogenation process. This work not only provides a new research direction in engineering efficient, low-cost catalysts for hydrogenation reactions, but also advances our understanding of hydrogen reaction paths.[1]

Exploring the interaction between two neighboring monomers has great potential to significantly raise the catalytic performance and deepen the mechanistic understanding of heterogeneous catalysis. Herein, we demonstrate the synergetic interaction between two neighboring Pt monomers on MoS_2 by facilely increasing the Pt mass loading up to 7.5% while still maintaining the atomic dispersion of Pt. In this case, Pt atoms replaced Mo atoms in MoS_2 nanosheets, wherein every Pt atom and its directly-bonded S atoms composed an “active center”. When two active centers were partly overlapped or adjacent, the two relevant Pt atoms were characterized as neighboring monomers. During CO_2 hydrogenation, the formation of neighboring Pt monomers significantly enhanced the catalytic activity and reduced the activation energy relative to isolated Pt monomers. Mechanistic studies reveal that neighboring Pt monomers not only worked in synergy to vary the reaction barrier, but also underwent distinct reaction paths compared with isolated monomers. Isolated Pt monomers favor the conversion of CO_2 into methanol without the formation of formic acid, whereas CO_2 is stepwise hydrogenated into formic acid and methanol for neighboring Pt monomers. The discovery of the synergetic interaction between neighboring monomers is expected to break a new path for manipulating their catalytic properties.[2]

Rh-based heterogeneous catalysts generally have limited selectivity relative to their homogeneous counterparts in hydroformylation reactions despite of the convenience of catalyst separation from the reaction mixture in heterogeneous catalysis. Here, we report a facile synthesis of CoO-supported Rh single-atom catalysts (Rh/CoO) with both remarkable catalytic activity and selectivity towards hydroformylation of propene. By increasing Rh mass loading, isolated Rh atoms switched to aggregated clusters of different atomicity. During the hydroformylation reactions, Rh/CoO achieved the optimal selectivity of 94.4% for butyraldehyde and the highest turnover frequency number of 2065 h^{-1} among the obtained atomic-scale Rh-based catalysts. Further mechanistic studies revealed that a structural reconstruction of Rh single atoms in Rh/CoO occurred during the catalytic process, facilitating the adsorption and activation of reactants. In terms of kinetics, linear products were determined as the dominating products by analyzing reaction paths deriving from the two most stable co-adsorbed configurations. As a bridge of homogeneous and heterogeneous catalysis, single-atom catalysts can be potentially applied in other industrial reactions.[3]

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A02-73

High-Capacity Electrode Materials for Advanced Lithium-Ion Batteries

Biao Gao*[1], Kaifu Huo[2]

1. The State Key Laboratory of Refractories and Metallurgy and Institute of Advanced Materials and Nanotechnology, Wuhan University of Science and Technology

2. Wuhan National Laboratory for Optoelectronics (WNLO), Huazhong University of Science and Technology Wuhan

With increasing demands of renewable energy, and hybrid electrical vehicles, high performance energy storage devices have attracted worldwide attention. Lithium-ion batteries (LIBs) have been intensively paid in energy storage due to their superior energy density, operating voltage and cycle life [1-5]. In order to satisfy the increasing demand for high energy density application, candidates with high theoretical specific capacity have proposed to replace commercial graphite as anodes due to its low theoretical specific capacity of only 372 mA h g^{-1}. Herein, we will introduce our recent work on the fbrication and Li ion storage properties of special nanostructures for high-performance LIBs anodes such as nitrogen-doped carbon hollow spheres, carbon conformal coating mesoporous hollow SiO_2 nanospheres, Si/C nanocomposites, conjointed Sn/C hollow spherical nanocomposite et. al [6-8]. Above nanostructured anodes with plentiful active sites for Li ion storage as well as the structural integrity exhibit high specific capacity and good cycling stability, enabling their promising applications in next generation LIBs.

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Keywords: Li ion batteries; Anodes; High capacity; Silicon; Tin

A02-74

Inorganic energy storage materials for new lithium air batteries

Jijing Xu*, Xiaoxue Wang, Lina Song, Fei Li, Lijun Zheng, Nan Luo
Jilin university

Lithium-air (Li-air) batteries is an attractive technology for electrical energy storage because of its high-energy density that is more than 10 times of lithium-ion battery. Its successful research and development will be a major breakthrough in energy history. However, the potential advantages of Li-air batteries are difficult to achieve, energy efficiency, rate capability, and cycle life are needed to be improved due to the problems of low positive reaction kinetics, slow mass transfer kinetics, poor electrolyte and anode stability, cathode passivation, etc. In response to these problems, we have designed and synthesized inorganic cathode materials such as series carbon modification and carbon substitution for inorganic energy storage materials for new lithium air batteries, which improve the electrochemical stability of the cathodes, thereby increase the specific capacity and cycle life; the prepared perovskite inorganic catalysts effectively reduce the charge/discharge overpotential of Li-air batteries, and significantly improve the energy conversion efficiency and rate capability; metal lithium anode prepared with lithium-fluoride polymer membranes for protection, which can effectively block the corrosion of anodes by substances such as oxygen and moisture in the air, while inhibit the growth of metal lithium dendrites and greatly increase the cycle life and safety.

Keywords: New inorganic energy storage materials; Lithium air battery; Energy storage mechanism; Air cathode

A02-75

Key Materials for Lithium Sulfur Batteries and Interface Modifications

Cheng Guo*, Huijun Yang, Jingyu Lei, Jiulin Wang
Shanghai Jiao Tong University

Lithium metal and elemental sulfur is the highest specific capacity solid materials, respectively. Therefore, lithium sulfur (Li/S) battery possesses the theoretical energy density up to 2600 Wh/kg and presents the next generation of batteries. Li/S also has obvious advantages of low cost and low or no toxicity. However, there several critical problems which prevent the Li/S for extensive applications. One is the very short cycle life and another lies in its high safety risk. Recently, there are various creative works which dramatically enhanced the electrochemical performances of sulfur cathodes and electrochemical performances of Li metal anode also have been obviously improved. The reported sulfur cathode materials can be divided into three main categories. The problems related to Li metal anode are serious dendrite, low Comlombic efficiency and obvious volume change.

Keywords: Li/S battery; S@pPAN; Li metal anode; Interface modification; Safety issue

A02-76

Activating and Templating of Zn to Synthesize Zn/N co-doped MoC Porous Nanosheets as Electrocatalyst for Efficient Electrochemical Hydrogen Evolution

Jianjian Lin*
NANJING TECH.

Developing non-precious metal catalysts with both high efficiency and durable stability is the top priority for hydrogen evolution reactions. Herein, we have developed a facile two-step method to synthesize Zn, N co-doped molybdenum carbide nanosheets (Zn-N-MoC-H NSs) by bi-metal oxides of $ZnMoO_4$. Zn not only serves as a template to form a porous structure on MoC nanosheets by volatilizing at high temperatures, but also as a doping source to regulate the electron density state of MoC thus enhancing the hydrogen evolution reaction (HER). Benefitting from the Zn/N co-doping, rich interfaces and the porous nanosheet structure with large electrochemical surface area, the Zn-N-MoC-H NSs exhibit excellent electrocatalytic activity in an acidic electrolyte (0.5 M H_2SO_4), with a low onset potential of −66 mV (1 mA cm^{-2}) and a small Tafel slope of 52.1 mV dec^{-1}, as well as

remarkable stability. As multifunctional catalyst, the obtained Zn-N-MoC-H NSs also possess high activity for water purification. This study offers an attractive electrocatalyst toward energy-efficient electrochemical production of hydrogen fuels, meanwhile, opens new avenues to explore the use of Zn as a nontoxic modulator toward high-efficiency catalysis and other applications of energy storage and conversion.

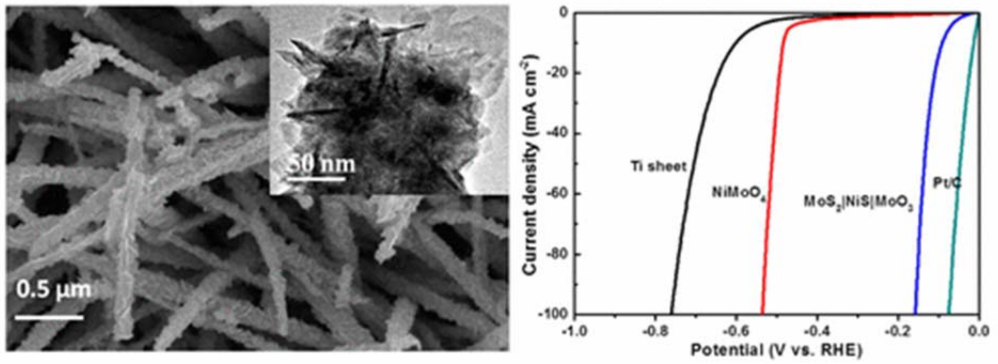
A02-77

Design and Synthesis of Synergistic Components for Electrocatalytic Water Splitting

Jiahai Wang*
1. Chemistry and Chemical Engineering Department, Guangzhou University
*Email: jiahaiwang@gzhu.edu.cn

A few researches have revealed that bicomponents possess much higher electrocatalttic activity as compared to single component. We have explored several systems to demonstrate the synergistic effect aroused from the interface between two components.

Keywords: Electrocatalyst; Water Splitting



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A02-78

Harnessing the concurrent reaction dynamics in active Si and Ge to achieve high performance lithium-ion batteries

Qiaobao Zhang*, Huixin Chen, Ming-sheng Wang
Xiamen University

Given its natural abundance, low average discharge potential (~0.4 V versus Li/Li+), and extremely high theoretical capacity of 4200 mAhg-1 (more than ten times that of the commercial graphite (372mAhg-1)), silicon (Si) has been regarded as one of the most promising anode candidates substituting for current commercialized graphitic anode for high-performance LIBs[1]. However, the dramatic volume expansion (>300%) and contraction of Si during lithiation/delithiation processes can cause a number of consequences including cracking and pulverization of Si anode, electrical disconnection from the current collector and destruction and regeneration of solid electrolyte interphase (SEI) layer on the fractured surfaces, which lead to rapid capacity fading and prevent it from being commercialized as LIBs anodes [1].

To solve these drawbacks, we report here the design of bamboo-like Cu/Si/Ge nanotube arrays with the highly conductive bamboo-like Cu as cores and Si and Ge as inner and outer shells that are directly grown on 3D porous Ni foam as high-performance LIBs anode materials. With this design, we have achieved a specific capacity high up to 955 mAh g −1 and about 71% capacity retention after 100 cycles at 0.2C of our electrode, suggesting good cycling stability.

Reference:
[1] Y. Sun, N. Liu, Y. Cui, Nature Energy, 2016, 13: 6071.

Keywords: Anode materials; Cu@Si/Ge nanowires; lithium-ion batteries

A02-79

Multiscale Simulaition Methods for Metal Nanoparticles in Operando Conditions

Beien Zhu*,Yi Gao

Shanghai Institute of Applied Physics， CAS

The catalytic reactions play the critical roles in the sustainable energy and environmental protection. The catalytic property of a nanoparticle is highly determined by its morphology. Recent developed in situ technology makes it possible to observe the structure reconstruction of nanoparticle under reaction conditions. The in situ studies of the dynamic structure evolution of nanoparticle in working conditions is very necessary to understand its actual activity. In recent works, we developed a Multiscale Structure Reconstruction Model (MSRM) for the metal nanoparticles under reaction conditions. Using our model, the shape evolution of various metal nanoparticles in water vapor, CO, NO, O_2, H_2 conditions have been quantitatively studied [1,2,3,4]. The theoretical results have extremely good consistency with experimental observations. Very recently, the support effects have been involved in our model [5]. We will show that our model can do multiscale, quantitative, and precise predictions. Moreover, an effective kinetic Monte Carlo simulation was developed to reproduce and explain the alloy transformation pathway observed in in situ experiments [6]. A software package of our model (MOSP) is now available for download and use.

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Keywords: structure reconstruction, in situ, multiscale modelling, nanocatalysts

A02-80

Construction of Surface Microstructure and Adjusted HER Catalytic Activity Sites for Molybdenum Carbide

Weijia Zhou*
South China University of Technology (SCUT)

Probing electrocatalysts for hydrogen evolution reaction (HER) is a hopeful approach to front the energy and environmental crisis[1]. Mo_2C is an efficient platinum-free-based electrocatalyst for HER. First, we synthesized Mo_2C on hierarchical porous carbon rods composed of cross-linked carbon networks using Cu-MoO_2 rods as Mo source and Cu template. The copper plays key roles in protecting Mo_2C from excess covering carbon to enhance the HER[2]. Second, ultrathin N-doped Mo_2C nanosheets were synthesized from MoO_2 nanosheets. Structural analyses make clear that the surfaces of N-Mo_2C NSs are encompassed of apical Mo atoms, hence affording an ideal prototype to expose Mo atoms for HER[3]. Third, we developed a two-step method to synthesize Zn, N co-doped η-MoC nanosheets by bi-metal oxides of $ZnMoO_4$. Zn not only serves as a template to form a porous structure on MoC nanosheets, but also as a doping source to regulate the electron density state of MoC thus enhancing the HER.

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A02-81

Interface Engineering in Planar Perovskite Solar Cells Within A Standard Structure

Chen Tao*
Wuhan University

The past 9 years has seen dramatic increases in the performance of perovskite solar cells (PSCs) with certified efficiencies over 20% that are approaching the level of Si solar cells. Although the standard meso-structured PSCs yeild higher efficiencies as well as less hysteresis, the high temperature involved meso-structured TiO_2 layer increases the fabrication cost and makes them not suitable on flexible plastic substrates. Therefore, standard PSCs with a planar structure are highly desired. However, it has been shown that the notorious hysteretic behavior prevents a correct evaluation of their potential. Hence, it is required to modify the interface between perovskite and the electron transport layer, which has been shown to be the main origin of hysteresis.

To address these issues, we will describe efficient planar methylammonium lead iodide ($CH_3NH_3PbI_3$) PSCs fabricated with two kinds of electron transport layer using fullerene derivatives,TiO_x/[6,6]-phenyl-C_{61}-butyric acid methyl ester (60-PCBM) and TiO_2/crosslinked [6,6]-phenyl-C_{61}-butyric styryl dendron ester(C-PCBSD) in conjunction with 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9-9'-spirobifluorene (spiro-MeOTAD)as the hole transport layer. The optimised TiO_x/60-PCBM with evaporation-solution hybrid processed $CH_3NH_3PbI_3$absorbing layers yields 17.6% stabilized efficiencies, while the TiO_2/c-PCBSD with all solution-processed $CH_3NH_3PbI_3$achieves efficiencies over 18%. They both significantly outperform their corresponding TiO_2-only references with less hysteresis. Perovskite deposited on fullerene derivatives presents larger-size grains with fewer boundaries. Photo-induced transient measurements show that the more efficient charge extraction and longer charge carrier lifetime in both 60-PCBM and C-PCBSD devices accounting for the higher power conversion efficiencies compared to the TiO_2-only references. Our results indicate that fullerene derivatives are a good candidate to be an electron transport layer in standard planarized PSCs. In particularly, the solution processed, robust TiO_2/C-PCBSD is well suited to high throughput, low cost all-solution processing PSCs.

A02-82

Study on thermoelectric properties of co-evaporated Sn-Se films with different phase formations

Baohai Jia*,Guojian Li,Shiying Liu,Shan Liu,Yongjun Piao,Qiang Wang
Northeastern University

The thermoelectric value (ZT) of SnSe single crystal can reach 2.6±0.3 at 923 K. Moreover, due to its abundant, non-toxic, and environment-friendly characteristics, SnSe has attracted wide attention. In this study, polycrystalline films with different SnSe and $SnSe_2$ contents were prepared by thermal co-evaporation of Sn and Se through adjusting their source temperatures and substrate temperature. The result shows that the pure SnSe film is p-type and consists by bulk-like nanoparticles, its resistivity is high up to 0.139 Ω·m, which causes poor thermoelectric performance. The films with two phases are made up of nanosheets. The $SnSe_2$ phase changes the conductivity type of the films and reduces the resistivity. At the same time, the $SnSe_2$ nanosheets perpendicular to the substrate and can improve the Seebeck coefficient of the film by filtering the low energy carrier. Compared with other samples, when the $SnSe_2$ content is 34%, the Seebeck coefficient of the film can reach 255 μV/K and the power factor can reach 155 μW/(m K^2) at 250 ºC.

Keywords: SnSe, film, thermoelectric, phase formation

A02-83

Gradient ultra-fine grained surface layer in 6063 aluminum alloy obtained by means of Rotational Accelerated Shot Peening

Ying Liu*[1], Hai Lu Xu[2], Yan Fang Liu[1], Zhong Cheng Liu[3]
1.School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing
2. PuJiang Institute, Nanjing Technology University, Nanjing
3. School of Mechanical Engineering, Nanjing University of Science and Technology, Nanjing

In view of the existing surface nano-technologies having many problems such as complex devices structure, small processing area and long processing time, etc, this paper proposes a new surface self-nanocrystallization devices, namely the Rotational Accelerated Shot Peening (RASP) surface treatment equipment. The technology uses turbine to accelerate projectiles to impact on the surface with a certain speed continuously, which produces strong plastic deformation in the surface to reach the purpose of grain refinement. This method is simple, safe and reliable with low cost of materials and equipment.

Mechanical properties of metallic materials improve after surface self-nano crystallization, such as strength, hardness, wear resistance and corrosion resistance. In this paper, by using RASP technique, gradient ultra-fine grained surface layer with a certain thickness was prepared for 6063 aluminum alloy. Moreover, optimum production technology parameters were obtained by changing the process parameters and orthogonal testing designation. The microstructure evolutions of the deformed surface layers were performed by TEM and other testing technology. The mechanical properties of samples were analyzed by means of portable roughness tester and hardness testing device .

The average grain sizes along the vertical section vary from hundreds of nanometers in the top surface to micrometers in the matrix. By using orthogonal experimental design to compare roughness values and hardness values, we synthesized the processing parameters to obtain sample of smaller roughness values and higher hardness.

Keywords: RASP; gradient ultra-fine grained structure; orthogonal experimental design; processing parameters

A02-84

A ternary ZnGeP2-TiC-C nanocomposite as large capacity and long lifetime anode for lithium ion batteries

Guoping Liu*[1], Zhicong Shi [1], Wenwu Li[1], Zaiping Guo[1,2]

1. Guangdong Provincial Key Laboratory of Functional Soft Condensed Matter, Smart Energy Research Centre， School of Materials and Energy, Guangdong University of Technology, Guangzhou 510006, China

2. Institute for Superconducting and Electronic Materials, Australian Institute for Innovative Materials, University of Wollongong, Innovation Campus, North Wollongong, NSW 2500, Australia

In conventional lithium ion batteries, graphite has been widely used as anode materials. However, the specific capacity of graphite is limited to 372 mAh g^{-1}, and the low intercalation potential of Li in graphite may cause safety problem due to the growing of Li dendrites[1]. Therefore, many efforts have been devoted to exploring alternatives for graphite, with the hope of simultaneously achieving large capacities and proper potential for Li$^+$ intercalation. Lithium alloying materials such as Zn, Ge and P have been wieldy investigated as potential candidates to meet this need due to their high theoretical capacities (based on the formation of LiZn, $Li_{4.4}Ge$ and Li_3P alloys) and higher operating potentials (vs. Li$^+$/Li) which grants greater safety from lithium plating during conditions of fast charge rate[1,2]. These elements have their own electrochemical characteristics in lithium storage. Zn, with the advantages of suitable lithium intercalation potential at average of 0.2 V (vs. Li$^+$/Li), possesses 4 voltage plateau owing to multi-phase changes during the lithiation process[3], which are unfavorable for kinetics of the lithium diffusion process. Ge has ultrahigh specific capacity because each atom can provide large amount of lithium storage of 4.4 Li, but the volume change of Ge during lithiation/delithiation process is up to 371%, resulting in the whole materials crack[4]. P can provide much higher intercalation potential of 0.7 V (vs. Li$^+$/Li) because the electronegativity of P is more negative and can help the reactivity of lithium electrochemical intercalation[5].

In this study, we synthesized $ZnGeP_2$ by a facile high energy mechanical ball milling of Zn, Ge and P. The electrochemical behavior of bulk $ZnGeP_2$ anode for lithium ion battery was investigated, and interesting phenomenon was found in the electrochemical reaction mechanism of lithium intercalation in $ZnGeP_2$ anode. The results show that the Li_5GeP_3, LiZnP, and Li_2GeZn intermediates, detected by ex-situ XRD during the cycling, have some special structures and properties that may help the diffusion of lithium in the bulk of active material during the cycling. In addition, we introduced TiC and C to synthesize $ZnGeP_2$-C, $ZnGeP_2$-TiC, and $ZnGeP_2$-TiC-C nanocomposite by high energy ball milling to improve the cycle performance of $ZnGeP_2$. The amorphous carbon acts as the buffer matrix to accommodate the stress induced by volume expansion during lithiation process. TiC, with properties of non-active and ultra-high hardness, can be used as the backbone to prevent the agglomerate of active matter during the cycling, and at the same time it acts as the milling aid to refine the grain size of active $ZnGeP_2$ that improve the electrochemical performance. With these merits, the $ZnGeP_2$-TiC-C anode exhibits an initial high specific capacity of 1521 mAh g^{-1} and a high initial coulombic efficiency of 93%. After 500 cycles the specific capacity still remains 1350 mAh g^{-1}.

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A02-85

Carbide (MxCy) derived functional nano-carbon electrocatalyst for oxygen reduction and hydrogen evolution reactions

Zongkui Kou, Wenqiang Li, Shichun Mu*

State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology

*Email: msc@whut.edu.cn

Metal- or semimetal (metalloid)-doped functional nano-carbon materials (graphene, carbon nanotube etc.) have been used to investigate new chemical properties for many fascinating applications in energy conversion and storage. However, the metal-doping into the nano-carbon structure is heavily hampered due to the obvious mismatching of lattices between carbon and metallic atoms (especially transition metal atoms). Thus, it is hard to realize the metal-doped functional nano-carbon material, and most of the preparation methods are still staying in the theory research.[1] Herein, we find a universal transformation of 2D carbides (MxCy) to few-layered graphene by the complete chlorination, and then obtain M-self-doped graphene/carbon nanotubes by tuning the chlorination process. The prepared Cr3C2 derived Cr-self-doped graphene and B4C derived B-self-doped carbon nanotubes present excellent oxygen reduction reaction (ORR) activity and stability in alkaline media. In addition, we first develop a novel “micro-cutting-fragmentation” technique by incomplete chlorination towards bulk TaC. Interestingly, benefiting from transition zones between in situ formed carbon layers and (222) facets, the evolution of high-index (222) facets with high surface energy can be prevented during preparation and electrochemical reaction. In the light of the highly generic nature, the methodology developed in this study can be widely applied to produce metal- or semimetal -self-doped functional nano-carbon materials and in situ synthesis of carbon armored high-index faceted metal carbide nanocrystals. These novel method s are readily scalable, opening a door to apply these materials to fuel cells and other fields.

Keywords: Nano-carbon, self-doping, metal, semi-metal, oxygen reduction, hydrogen evolution

Reference: [1] Kang H S. J. Am. Chem. Soc. 2005, 127(27): 9839.

墙展

A02-P01

Nanocellulose/conductive polymer aerogel electrodes for supercapacitor application with higher conductivity and capacitance via adding vapor grown nano-carbon fiber as conducting networks

Yanping Chen [1,2]， Shaoyi Lyu [1]， Shenjie Han [1]， Limin Guo [1], Wenjun Wang[2], Siqun Wang[3,1]
1.Research Institute of Wood Industry, Chinese Academy of Forestry, Beijing 100091, China
2.Beijing Engineering Research Center of Cellulose and Its Derivatives, School of Materials Science and Engineering, Beijing Institute of Technology, Beijing 100081, China
3.Center for Renewable Carbon, University of Tennessee, Knoxville, Tennessee, 37996, USA

Nanocelluloses based conductive materials have been widely studied as electrode of wearable supercapacitors. Herein to obtain electrode materials with higher conductivity and capacitance, conductive polymer (polypyrrole andpolyaniline) were in situ polymerized based on cellulose nanofibrils (CNF) and vapor grown nano-carbon fibers (VGCF) hybrid aerogels. The conductivity of CNF/VGCF aerogel has been improved greatly after adding VGCF and increased with the increased content of VGCF, which is beneficial for transfer of electron and reducing inter resistance. In addition, the capacitance of the electrode materials was improved as result of synergistic effects caused by double-layer capacitance of VGCF and pseudocapacitance of conductive polymer in CNF/VGCF/conductive polymer aerogels. Therefore, CNF/VGCF/conductive polymer aerogel electrode materials showed higher capacitance. All-solid-state supercapacitor fabricated by the above electrode materials showed higher energy density and power density, providing great potential for use in supercapacitors or other electronic devices with good electrochemical properties.

Keywords: cellulose nanofibrils, vapor grown nano-carbon fibers, supercapacitor, aerogel

A02-P02

CsPbBr3 Nanocrystals Embedded in Cs4PbBr6 Host Matrices: Ion Concentration Difference Induced Formation and Application in White Light-Emitting Diodes

Wenkang Wang*[1], Tianjin Zhang[1], Duofa Wang[1], Song Wang[2]
1. Hubei University
2. Hubei University of Arts and Science

The poor stability of perovskite nanocrystals (NCs) hinders their potential application in photoelectronics. Here, we develop a self-assembly reaction to fabricate $CsPbBr_3$ NCs embedded in a host Cs_4PbBr_6 matrix at room temperature. *In-situ* characterization reveals that the $CsPbBr_3$ NCs/Cs_4PbBr_6 matrix structure is formed by a two-step reaction, driven by ion concentration difference. The self-encapsulation and separation of the $CsPbBr_3$ NCs by the host Cs_4PbBr_6 result in the material exhibiting a high PLQY of 56% and narrow-band emission at 517 nm with a full width at half-maximum of only 21 nm. Further, we fabricate an on-chip white light-emitting diode (LED) using the as-synthesized $CsPbBr_3/Cs_4PbBr_6$ nanocomposites as a green emitter and red $K_2SiF_6:Mn^{4+}$ phosphor on the surface of a blue LED chip. The resulting white LED exhibits a high luminous efficiency of up to 43.22 lm W^{-1} at 20 mA with an NTSC value of 131% and Rec. 2020 of 98%. These $CsPbBr_3/Cs_4PbBr_6$ nanocomposites show great potential application in white LED, due to their outstanding performance as well as environmentally friendly, facile, and applicable for mass production fabrication method.

Keywords: $CsPbBr_3/Cs_4PbBr_6$ nanocomposites, all-inorganic perovskite, LED

A02-P03

Efficient hydrogen isotopologues separation through a tunable potential barrier: The case of a C2N membrane

Yuanyuan Qu*[1], Feng Li[1,2], Mingwen Zhao[1]
1. Shandong University
2. University of Jinan

Isotopes separation through quantum sieving effect of membranes is quite promising for industrial applications. For the light hydrogen isotopologues (eg. H_2, D_2), the confinement of potential wells in porous membranes to isotopologues was commonly regarded to be crucial for highly efficient separation ability. Here, we demonstrate from first-principles that a potential barrier is also favorable for efficient hydrogen isotopologues separation. Taking an already-synthesized two-dimensional carbon nitride (C_2N-*h*2D) as an example, we predict that the competition between quantum tunneling and zero-point-energy (ZPE) effects regulated by the tensile strain leads to high selectivity and permeance. Both kinetic quantum sieving and equilibrium quantum sieving effects are considered. The quantum effects revealed in this work offer a prospective strategy for highly efficient hydrogen isotopologues separation.

Keywords: two-dimensional carbon nitride, quantum sieving, isotopes separation, hydrogen separation

A02-P04

A new approach to produce a nanocrystalline layer on surface of a large size pure titanium plate

Quantong Yao*
Northeastern University

It was demonstrated that the mechanical shot peening (MSP) technique was a feasible method for producing a nanocrystalline layer on a large size pure titanium plate due to the MSP provided for severe plastic deformation (SPD) of surface via high velocity balls impacting. The MSP effects of various durations in producing surface nanocrystalline layer was investigated by optical microscope (OM), X-ray diffraction (XRD), transmission electron microscope (TEM), and Vickers micro-hardness tester. The experimental results showed that the thickness of SPD layer gradually increased with the MSP processing time prolong, but obtained stability of 230 μm after 30 min. The average grains size was refined to about 18.48 nm in the naonocrystalline layer. The grains in the topmost surface presented equiaxed grain morphology with random crystallographic orientation. By comparing with the nanocrystalline layer produced by SMAT, the microstructure and properties of the nanocrystalline layer produced by MSP was evidently superior to that of the SMAT, but the production time was cut to about a quarter of the SMAT method.

A02-P05

Thermal stability and photocatalytic activity of highly ordered anodized TiO2 nanotube arrays with interstitial nitrogen as dominant point defect

Qing Ma*[1,2], Zhiyuan Luo[3], Shang Gao[3], Dingning Ke[1], Ting Kuang[1], Linlin Song[1], Shishan Ji[2]
1. Experiment and Innovation Center, Shenzhen Graduate School, Harbin Institute of Technology
2. Research Institute of Tsinghua University in Shenzhen
3. Department of Materials Science and Engineering, Shenzhen Graduate School, Harbin Institute of Technology

High ordered TiO_2 nanotube arrays (TNTs) with interstitial nitrogen as dominant point defect have been successfully synthesized by annealing as-anodized TNTs in N_2 at temperatures with a temperature range from 400°C to 650°C for 1h. It is shown by FESEM, XRD, and Raman spectroscopy that the thermal stability of TNTs annealed in N_2 is higher than that of TNTs annealed in

O_2. In contrast, it is lower than annealed TNTs in NH_3. The interstitial nitrogen is considered as the dominant point defect in TNTs annealed in N_2, which result in the significantly improved thermal stability of highly ordered TNTs. However, the concentration of hydroxyl oxygen on the surface of TNTs is significantly influenced by annealing temperature, which is closely related to the photocatalytic activity. The optimized photocatalytic activity of photo-degradation of MO with pseudo-first-order reaction constant k value of $(5.065\pm0.139)\times10^{-2}\ h^{-1}$ is achieved for TNTs annealed in N_2 at 600°C . These findings could provide a simple but versatile method to fabricate highly ordered TNTs with controllable point defects, enhanced thermal stability, and photocatalytic activity.

Keywords: Thermal stability; Photocatalytic activity; Interstitial nitrogen; TiO_2 nanotube arrays

A02-P06

Synthesis of Open Helmet-Like Carbon Skeletons for Application in Lithium-Ion Batteries

Wentao Jing*
Wentao Jing

How to optimize the interior spaces of symmetric (for example, hollow carbon spheres) and asymmetric (for example, hollow carbon bowls) hollow carbon structures is a big challenge for their applications in energy storage devices. Here we synthesize open helmet-like carbon skeletons, carbon nanohelmets (CNHs), which reserve all advantages of hollow structures but also fully utilize the inner walls of carbon. As an example, the as-fabricated NiO/CNHs anode exhibits high reversible capacity, excellent cycling stability and superior rate property in lithium-ion batteries. These remarkable performances are attributed to the ingenious helmet-like structures, which provide a large amount of active sites for Li+ insertion/extraction from inner walls of carbon; buffer the large volume change of NiO during charging/discharging effectively with the open structure; and reduce the internal resistance significantly due to excellent contact between NiO nanoparticles and carbon. The facial strategy reported in this work may open an avenue to synthesize open hollow structures for practical applications.

A02-P07

Super-sensitive O_2 gas sensor based on La-SnO_2 nanofibers through temperature modulation

Ya Xiong*, Hui Li, Tianchao Guo, Qingzhong Xue
China University of Petroleum

Generally sensing mechanisms of gas sensors greatly depend on temperature, and this is particularly true for metal-oxide semiconductors based sensors where the peculiar role of temperature suggests temperature modulation can be applied as a vital method to effectively enhance the sensor response. In this paper, we reported a breakthrough of quick-cooling operation mode in the course of gas sensing process to elevate the O_2 response while maintaining low heating energy consumption. La-SnO_2 nanofibers synthesized by electrospinning were chosen as gas sensing materials. The responses toward O_2 gas by employing quick-cooling operation mode are significantly improved compared with those obtained by traditional isothermal test. The strategy demonstrated here could also be extended to other gas sensor as long as its response with respect to gas concentration is a function of the sensor temperature.

Keywords: Electrospinning; La-SnO_2 nanofibers; O_2 gas sensor; Quick-cooling operation mode

A01-P08

Preparation of b-oriented MFI zeolite films in neutral synthesis condition

Yong Peng*
College of Science, Nanchang Institute of Technology

Objectives: MFI zeolite films and membranes have found many applications in the field of separation, catalysis, sensors, and corrosion-protection. One particularly interesting but challenging issue is the fabrication of dominantly *b*-oriented pure silica MFI zeolite films. Generally, *b*-oriented MFI zeolite films are prepared in the alkaline synthesis condition by secondary growth method. In order to prevent Al leaching from the porous alumina supports, an intermediate silica layer should be precoated on the support surface. This process is tedious and requires additional treatment steps prior to membrane synthesis. New synthesis technique utilizing neutral or near-neutral synthesis solutions is an attractive alternative. At present, HF was usually used in the preparation process. Handling of HF is highly undesirable due to its corrosiveness. Therefore, the exploration of a new neutral synthesis method without the need of HF is highly desired. In this abstract, we demonstrate that under the neutral synthesis system of TPABr/fumed

silica/H_2O, *b*-oriented MFI films can be facilely synthesized on the support of glass plate.

Methods: Glass plates were immersed in hydrogen peroxide solution for 45 min, then rinsed with deionized water, and dried at 60 °C before the synthesis of zeolite films. Tetrapropylammonium bromide (TPABr, 99%) was purchased from Sinopharm. Fumed silica (99.8%) was purchased from Xi'ya Reagent. Perfectly *b*-oriented MFI seed monolayers were prepared on the supports of glass plates by rubbing MFI zeolite crystals with a finger in latex glove. The seeded support was vertically placed in a Teflon-lined stainless steel autoclave for secondary growth. The synthesis solution was made by slowly adding fumed silica to a solution of TPABr and water under stirring. The molar composition of the resulting gel was 0.1TPABr : (0.1 ~ 2.0)SiO_2 : 165H_2O. The gel was aged for 1 h prior to use at room temperature. The seeded growth was carried out at 175 °C for 12 to 24 h. After synthesis, the film was rinsed with deionized water and dried at 60 °C. The top and cross-sectional images of the zeolite films were observed using scanning electron microscope TM-1000 and SU-70 (Hitachi). X-ray diffraction (XRD) patterns were collected on a PANalytical X'PertPro diffractometer using Cu *Kα* radiation.

Results: We first tried the synthesis solution with the composition of 0.1TPABr : SiO_2 : 165H_2O ($TPA^+/Si = 0.1$) for the secondary growth. Fumed silica was used as the silica source. The synthesis solution is neutral since no other chemical reagent is added. SEM was used to charactrize *b*-oriented MFI zeolite seed layer on glass plate prepared by hand-rubbing and the evolution of zeolite film morphology along with the crystallization time. It is seen that a long crystallization time is favorable for the improvement of continuity of the zeolite film. A continuous and twin-free *b*-oriented zeolite film can be achieved when the time is prolonged to 24 h. The crystal size along *c*-axis is increased to about 2.4 μm from 1.0 μm and the thickness of the film is about 380 nm after the synthesis of 24 h. Crystallization time less than 24 h is not adequate for the formation of continuous films. The crystal size is slightly increased to 1.6 μm and 2.0 μm after secondary growth for 12 h and 18 h, respectively. To analyze the channel orientation, the zeolite films were examined by X-ray diffraction. The diffraction patterns of the seed layerand zeolite films only show the diffraction peaks from the (020), (040), (060), (080), and (0100) planes, confirming that the synthesized films are highly *b*-oriented. When the molar amount of silica source in the synthesis solution was decreased to 0.1 and 0.5 (i.e., the synthesis solution composition is 0.1TPABr : 0.1SiO_2 : 165H_2O and 0.1TPABr : 0.5SiO_2 : 165H_2O), the synthesized *b*-oriented zeolite films are still continuous. The crystal size of zeolite film synthesized in lower silica ratio (3.6 μm) is even larger than that obtained in higher silica ratio (2.4 μm). Despite the TPA^+/Si ratio is 1.0, no clear twin crystals can be observed on the zeolite film. XRD patterns suggest that the synthesized MFI zeolite films are still highly *b*-oriented when altering the molar ratio of fumed silica of the synthesis solution composition. By contrast, increasing the amount of fumed silica has no promotion effect on the crystal size of zeolite film.

Conclusions: We developed a neutral synthesis solution system without fluoride for the preparation of highly b-oriented MFI zeolite films. When using glass plates as film supports, the dissolved Na_2O from the glass plate facilitate the secondary growth of MFI seed crystals in the synthesis system of TPABr/fumed silica/H_2O. The novel neutral synthesis system may provide us a new route for the direct synthesis of b-oriented MFI zeolite films and membranes on various substrates.

Keywords: zeolites, thin films, oriented film, MFI, hydrothermal synthesis

A01-P09

Superior energy storage performance achieved in bismuth ferriete-based film capacitors via domain engineering

Hao Pan*[1], Jing Ma[1], Ji Ma[1], Qinghua Zhang[2], Lin Gu[2], Yang Shen[1], Yuan-Hua Lin[1], Ce-Wen Nan[1]

1. State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering， Tsinghua University, Beijing 100084, P. R. China.

2. Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, P. R. China.

Developing high-performance film dielectrics for capacitive energy storage has been a great challenge for modern electrical devices. Despite good results obtained in lead titanate-based dielectrics, lead-free alternatives are strongly desirable due to environmental concerns. Here 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 lead-free bismuth ferrite-strontium titanate solid-solution films through domain engineering. It is revealed that the incorporation of strontium titanate transforms the ferroelectric micro-domains of bismuth ferrite into highly-dynamic polar nano-regions, resulting in a ferroelectric to relaxor-ferroelectric transition with concurrently improved energy density and efficiency. Additionally, the introduction of strontium titanate greatly improves the electrical insulation and breakdown strength of the films by suppressing the formation of oxygen vacancies. This work opens up a feasible and

propagable route, i.e., domain engineering, to systematically develop new lead-free dielectrics for energy storage.

A01-P10

Mo_2C on Carbon Fiber Paper synthesized in Molten Salt for Hydrogen Evolution Reaction

Wenjin Yuan*[1,2], Nianxiang Qiu[2], Qin Huang[2], Zhenduo Cui[1], Shengli Zhu[1], Zhaoyang Li[1], Yanqin Liang[1]
1. School of Materials Science and Engineering, Tianjin University, Tianjin
2. Engineering Laboratory of Nuclear Energy Materials, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences

Many efforts are made to develop effective electrocatalysts and modifying them by means of structure regulation, doping, etc. However, investigations about the effects of different crystal faces on catalytic performance are rare. Herein, we propose an one-step synthetic method to grow (100) plane oriented Mo_2C on carbon fiber paper in a molten salt system. The electrocatalytic properties towards hydrogen evolution reaction (HER) show that (100) plane oriented Mo_2C functions well in both acidic and basic media. It is revealed to exhibit an overpotential (η_{10}) of 170 mV at -10 mA cm^{-2} in acidic medium (pH = 0) and η_{10} of 95.8 mV in alkaline medium (pH =14), which is more active than common Mo_2C. The further density function theory calculations show that the hydrogen adsorption free energy (ΔG_{H*}) of (100) plane of Mo_2C is -0.066 eV, suggesting a good balance between Volmer and Heyrovsky/Tafel steps in HER kinetics.

A01-P11

MoSe2 nanosheets grown on graphite as effective catalytic hydrogen evolution electrodes

Xu Mao*, Jianpeng Zou, Danni Li
State Key Laboratory of Powder Metallurgy, Central South University

The growing demands of energy and higher requirements in environmental protection in modern society have prompted us to constantly search for low-cost and sustainable energy sources. Hydrogen (H_2) is a kind of sustainable and pollution-free energy which plays a vital role in fuel cells. Electrochemical water splitting is an excellent eco-friendly approach to produce hydrogen gas with massive scale. The major challenge in hydrogen evolution reaction (HER) is the demand of earth-abundant and inexpensive catalytical materials with commendable catalytic activity to replace the scarce and costly platinum electrode. $MoSe_2$ films with perpendicular texture were synthesized on inexpensive graphite substrate for catalytic application in the hydrogen evolution reaction. Mo nanofilms with a thickness of about 50 nm were deposited onto the graphite substrate by direct-current magnetron sputtering. The Mo/graphite film was heat-treated in selenium vapor in horizontal tube furnace to form $MoSe_2$/graphite composite electrode. The hydrogen evolution reaction activity of the electrode was evaluated by linear sweep voltammetry. Scanning electron microscopy and Raman spectroscopy indicated that the graphite substrate was covered with $MoSe_2$ nanosheets tightly. The size, number and crystallinity of $MoSe_2$ nanosheets can be controlled by adjusting the selenization parameters to achieve better HER activity of the electrodes. $MoSe_2$/graphite electrodes prepared at 500 ℃ for 15 min exhibit the best HER activity and great stability in acidic solution with an over potential around 125 mV vs reversible hydrogen electrode (RHE) at the current density of 10 mA cm^{-2}. The Tafel slope of $MoSe_2$/graphite electrodes is 52.10 mV dec^{-1}, which shows the best performance among the reported literatures of $MoSe_2$ materials. Vertical aligned $MoSe_2$ nanosheets contribute to the exposure of active catalytic sites and the observed HER performance in this study is among the best reported to date.

A01-P12

Synthesis of hierarchical Cd0.65Zn0.35Te nanostructures via self-assembly of quantum dots

Wangwei Lu*, Gaoling Zhao, Gaorong Han
School of material science and engineering, Zhejiang University, Hangzhou 310027, China

Quantum dots (QDs) are attracting more and more scientific attention due to band gap tunability, high absorption coefficient, and solution process ability. However, their applications are limited due to short carrier diffusion lengths of quantum dots. This generally leads to carrier recombination before the electron transport, and thus a significant decrease in the efficiency of the photovoltaic conversion. Therefore, developing quantum dots with long carrier diffusion lengths is critical for their application. In present work, hierarchical $Cd_{0.65}Zn_{0.35}Te$ nanostructures were prepared by a self-assembly route. X-ray photoelectron spectrometer

ensured that the composition of Zn and Cd in the quantum dot was $Cd_{0.65}Zn_{0.35}Te$. The X-ray diffraction (XRD) patterns confirmed the cubic zinc blende structure of $Cd_{0.65}Zn_{0.35}Te$ nanostructures. Scanning electron microscopy (SEM) images showed that the $Cd_{0.65}Zn_{0.35}Te$ nanostructures were composed of interconnected nanorods. Transmission electron microscope (TEM) revealed that the interconnected $Cd_{0.65}Zn_{0.35}Te$ nanorods were self-assembled by $Cd_{0.65}Zn_{0.35}Te$ QDs. The particle size of $Cd_{0.65}Zn_{0.35}Te$ QDs were about 3.0 nm. Carrier diffusion lengths of $Cd_{0.65}Zn_{0.35}Te$ nanostructures were increased greatly compared with $Cd_{0.65}Zn_{0.35}Te$ QDs, due to their branched networks, which was confirmed by the photoluminescence (PL) decay measurement. In addition, no obvious shifts in absorbance peaks and fluorescence peaks of $Cd_{0.65}Zn_{0.35}Te$ nanostructures were observed, indicating that the size of $Cd_{0.65}Zn_{0.35}Te$ QDs were mostly retained in self-assemble process.

A01-P13

SERS performance of β-Sn/rGO hybrid structure

Hanhan Wu*, Bin Li, Hong-Hai Zhong, Ying-Wei Lu
Hefei University of Technology

Noble metal, such as Au and/or Ag, nanoparticles have been widely employed as substrates for surface enhanced Raman scattering (SERS) because of their fantastic localized surface plasmon performance with extremely high enhancement factors (EF). Unfortunately, bare metallic substrates suffer from problems including poor stability and reproducibility due to their aggregation. The noble metal/graphene hybrid substrates therefore have been attracted tremendous interests to make up the deficiency of traditional plasmonic metal substrates, since graphene can improve the ability to adoption of target molecules thanks to its unique physical and chemical properties. However, the electronic heterogeneity between the noble metals and graphene will result in some electronic defects which could reduce the EF dramatically.

Herein, we designed a novel β-Sn/rGO hybrid plasmonic nanostructure and fabricated it through a solvothermal route. In this typical procedure, GO was dispersed in ethanol with ultra-sonication for 1 h. The β-Sn/rGO composite was subsequently synthesized at high temperature for 6 h in the Teflon lined stainless steel autoclaves by using PVP and NaBH4 as dispersant and reducing agents, respectively.

The formation of Sn nanoparticles with an average size of 30 nm dispersing on rGO sheet have been observed by a FETEM. Furthermore, the composition of such hybrid have been confirmed by XRD, EDS mapping and Raman characterizations. Most importantly, an ultrasensitive detection limit of rhodamine-6G (R6G) as low as 10-3 M have been achieved, which can be attributed to the synergistic effect of the β-Sn/rGO nanocomposite including the chemical enhancement and the near field effect resulting from rGO and the β-Sn nanoparticles, respectively. In addition, the local electric field strength and distribution of such hybrid structure have been simulated by a finite element method, and the results indicate that the theoretical EF of SERS agree with the experimental values very well.

In summary, a novel β-Sn/rGO hybrid plasmonic nanostructure was prepared successfully. The combination of β-Sn nanoparticles and rGO could act synergistically to achieve higher Raman signals comparing with either bare rGO or bare β-Sn nanoparticles.

A01-P14

The effects of reductive degree of graphite oxide on the visible-light-driven photocatalytic activity of $MnWO_4$ for water splitting

Hongru Zhou*, Yuanyuan Peng, Jun Ke
Wuhan Institute of Technology

As an important half reaction in solar-driven water splitting, it is still a challenging issue to develop low-cost and high efficient photocatalysts for water oxidation process. In this paper, ternary metal oxide $MnWO_4$ nanobars is coupled with layered reduced graphene oxide (rGO) to construct rGO/$MnWO_4$ heterojunctions for enhancing photocatalytic water oxidization activity under visible light irradiation. The uniform $MnWO_4$ nanobars and 2D layered graphite oxide (GO) were firstly synthesized via hydrothermal process and modified Hummer's method, respectively. After that, a series of rGO/$MnWO_4$ composites were prepared by using different reductive reagents (water, ethanol, L-ascorbic and hydrazine hydrate) through second hydrothermal process for photocatalytic O_2 evolution. As a result, the rGO prepared by using water and ethanol as reduction reagents possesses low reductive degree and dramatically undermine the photocatalytic activity of $MnWO_4$, which indicates that the reduction of graphene oxide plays a key role in raising photo-induced charge carrier separation efficiency as an electron collector through the interaction between rGO and $MnWO_4$. It is speculated that the oxygen-containing groups at the edge of the layered graphene oxide can obstruct immigration of photoinduced charge carries at between $MnWO_4$ and graphene, leading to the severe recombination of electrons and holes. These results could provide a new idea to regulate the behavior of photogenerated charge carriers in graphene-based photocatalysts for improved separation efficiency of electron and holes and enhanced photocatalytic water splitting activity.

A01-P15

Two-Step Vapor Deposition of Self-Catalyzed Large-Size PbI2 Nanobelts for High-Performance Photodetectors

Mingming Han*, Zai-xing Yang
Shandong University

The grown lead iodide (PbI_2) is usually two-dimensional sheets with a finite size which necessitate sophisticated device metallization and the growth of quasi one-dimensional materials is still challenging. In this work, large-size (length > 100 μm), single-crystalline and high-density PbI_2 nanobelts are successfully synthesized by manipulating the microenvironment in a two-step vapor deposition process at a slow heating rate of ~18 oC min-1. Firstly, PbI_2 nanosheet seeds are grown by physical vapor deposition, and then PbI_2 nanobelts are synthesized by a self-catalyzed vapor-liquid-solid growth mechanism, which is verified by the Pb nanoparticles on the nanobelts tips. Photoluminescence and ultraviolet-visible spectra show the uniform high-quality crystallinity of the as-prepared large-size PbI_2 nanobelts with a bandgap of 2.36 eV. When configured into photodetectors with a shadow mask, the fabricated device exhibits a low dark current of 4 pA, an impressive ON/OFF current ratio of 103 ~ 104, a photoresponsivity of 13 mA W-1, and a fast response with the rise and decay time constants of 425 and 41 ms, respectively. All these performances are comparable to those of state-of-the-art of layered PbI2 nanostructures photodetectors, but the ease of synthesizing large-size PbI2 nanobelts may have useful impact on next-generation easily-fabricated high-performance optoelectronics.

A01-P16

Preparation and enhanced photoelectrocatalytic activity of ternary TiO2-Fe2O3/Cu Nanocomposites

Hexi Zhao*, Huiyuan Chen, Hui Nan
Qinghai University

TiO_2-Fe_2O_3/Cu nanocomposite was successfully synthesized via a hydrothermal method. The morphology, structure and photocatalytic activity were characterized by means of X-ray diffraction(XRD), scanning electron microscope(SEM), transmission electron microscope (TEM), X-ray photoelectron spectroscopy(XPS), Fourier transform infrared spectroscopy (FT-IR), UV-vis diffuse reflectance spectra(UV-vis DRS), Cyclic voltammograms (CV), Electrochemical impedance spectroscopy (EIS) and Tafel polarization curve(Taf). The photocatalytic performance of Fe_2O_3, TiO_2, TiO_2-Fe_2O_3 and TiO_2-Fe_2O_3/Cu for degradation of methyl orange (MO) were explored under UV−Vis irradiation.UV−Vis diffuse reflectance spectrum was used to measure the optical absorption property of the samples.

The results shown that TiO_2-Fe_2O_3/Cu nanocomposite exhibited the best photocatalytic activity due to the improved light utilization and charge transfer property,which is related to the charge transfer resistance of TiO_2 > Fe_2O_3 > TiO_2-Fe_2O_3 > TiO_2-Fe_2O_3/Cu in EIS snd Taf. At the same time,for TiO_2-Fe_2O_3/Cu nanocomposite decomposing MO,the degradation kinetics is faster than other samples at the same condition.

A01-P17

Control of microstructure and properties of graphene aerogel via manipulation of ice crystal template by freeze-casting

Xiangyu Zhu*[1], Pingwei Wu[2], Hailong Zhang*[1]
1. State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, China
2. School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China

Graphene aerogel (GA) is one of the most attractive graphene-derived 3D materials and has demonstrated great potential in many fields. However, it is still a challenge to precisely tailor the pore structure of GA to fit in versatile application backgrounds. In this study, the effects of ice crystals on microstructure and properties of GA during freeze-casting were systematically investigated. The results suggest that the freezing rate is the key to controlling the nucleation and growth of ice crystals and dominating the morphology of GA. Rapid freeze-casting endows the GA better thermal, electrical and compressive properties because of the refined pore structure, whereas the GA frozen at high temperature has superior absorption properties owing to the continuous and tube-like graphene lamellae. There is a strong link between the freezing temperature and the properties of graphene aerogel, which helps not only the production of GA under different application backgrounds but also paves the way for other cryogenic induced phase separation methods.

A01-P18

Cost-effective Ag nanorods/rGO for oxygen reduction in alkaline medium

Dongxiang Zhu*, Ji-Gui Cheng, Ying-Wei Lu
HeFei University of Technology

Nowadays, platinum (Pt) or platinum alloys are the most advanced electrocatalysts for oxygen reduction reaction (ORR) and play a crucial role in fuel cells, which is one of the popular new energy devices. However, the high cost of precious metals is one of the obstacles to the commercialization of fuel cells. Recently, it has been proven that carbon supported Ag nanostructures could be an alternative effective ORR catalyst since the Ag nanostructures present reasonable activity and stability and the carbon substrate could help Ag to achieve uniformly dispersion and high migration rate of electrons. As a result, Ag/reduced graphene oxide (Ag/rGO) nanohybrids become one of the most promising ORR catalysts and have been attracted intense attention.

In this work, a green, convenient and cost-effective electrochemical method was employed to simultaneously reduce Ag ions and GO to obtain Ag nanorods uniformly dispersing on rGO sheets. In this case, GO coated Si wafer and graphite plate were used as electrodes immersing in $AgNO_3$ solutions with different concentrations to get different nanohybrids. While the voltage was kept at 3 V during the reduction.

The morphologies and compositions of synthesized nanohybrids had been confirmed by TEM, XRD, XPS and Raman characterizations. The kinetic parameters of the as-prepared catalysts were determined using the rotating disk electrode technique, and the linear sweep voltammetry were measured in O2-saturated 0.1 M KOH solution at 1600 rpm. For comparison, a commercial carbon-supported Pt catalyst (Pt/C) was investigated under the identical conditions as well. The results reveal that both the onset potential (0.895 V) and the limiting diffusion current density (5.72 mA/cm^2) of Ag/rGO samples are comparable to those of Pt/C catalyst implying a reasonable high ORR activity. Such fantastic ORR performance could result from the high catalytic activity of the Ag nanorods and the excellent electron transfer properties of rGO. In addition, the decreasing of oxygen-containing groups on the surface of rGO is beneficial to improve the ORR activity of Ag/rGO catalysts.

In conclusion, Ag nanorods/rGO nanohybrids have been successfully obtained by a facile electrochemical method and the measurements indicate that such nanohybrids could act as a low cost catalyst for ORR in fuel cells with similar performance to commercial Pt/C catalyst.

A01-P19

Controlled aqueous synthesis of noble metal/semiconductor hybrid nanocrystals and their applications

Xinyuan Li*[1], Meng Xu[1], Hongzhi Wang[1], Muwei Ji[2], J iatao Zhang[1]
1. Beijing Institute of Technology
2. Graduate School at Shenzhen, Tsinghua University

The integration of different components into one hybrid nanostructure with controlled morphology, size and interior voids is important to get flexible and cooperative coupling between different properties, in particular the case of semiconductor/semiconductor and metal/semiconductor hybrid nanostructures. Hybrid nanocolloids with programmed three-dimensional shape and material composition towards system materials engineering become a new trend. Cation-exchange reactions in colloidal nanocrystals (NCs) are regarded as efficient strategies to versatile fabricate high crystallization NCs at acceptable experimental conditions. However, the aqueous cation-exchange reactions beyond quantum sized (over 30 nm) were lack of studied. Herein, we put forward an aqueous synthesis strategy by carefully sulfuration of as-prepared cavity-free core/shell NCs or metal oxide NCs and then phosphine initialized cation exchange reactions to prepare metal@semiconductor and metal oxide@semiconductor (II-VI) yolk-shell NCs. Besides, by introducing core-shell Au@Ag_3AuTe_2 as intermediate phase, aqueous cation-exchange between core-shell Au@Ag_2Te and Au@CdTe NCs was systematically studied and Au@CdTe NCs with high crystallization were achieved. Further cation-exchange reaction was also applied to unprecendentedly synthesize Au@HgxCd1-xTe

NCs. Tunable optical absorption was achieved by precisely controlling the element ratio, shell thickness and morphologies of plasmonic cores. We believe that the proposed synthesis strategy could be extended to further aqueous cation-exchange reactions and the as-prepared NCs could be proper candidates for optoelectronic applications.

A02-P20

Effect of Annealing on the Magnetic Properties of FeCoNiCuNbSiB Soft Magnetic Alloys

Zhun Li*[1], Kefu Yao[2], Deren Li[1], Zhichao Lu[1]
1. Advanced Technology and Materials Co., Ltd
2. Tsinghua University

A series of $Fe_{66.8-x}Co_{10}Ni_xCu_{0.8}Nb_{2.9}Si_{11.5}B_8$ (x=1-15 at. %) nanocrystalline soft magnetic alloys with low permeability were synthesized by adjusting Ni content. Effect of annealing on the soft-magnetic properties, crystallization behavior and microstructure were investigated. It is found that the temperature interval between the two crystallization peaks is significantly decreased from 162 to 100 ℃ when the Ni content of the alloys increases from x = 1 to x = 15, which greatly reduces the optimum annealing temperature range. The alloys with higher Ni content are prone to exhibit lower permeability, and the Fe-based FeCoNiCuNbSiB nanocrystalline alloys with x = 15 exhibit excellent soft-magnetic properties, including the low permeability of 2000, low coercivity of about 0.6 A/m and low remanence of 2.4 mT. The combination of low permeability and excellent soft-magnetic properties makes the FeCoNiCuNbSiB nanocrystalline alloys to be a kind of promising material for common mode chokes and current transformer with direct current tolerance.

A02-P21

Tuning the Electronic Structure of NiO via Li doping for Fast Oxygen Evolution Reaction

Gaoliang Fu*, Xiaojian Wen, Jun Cheng, Kelvin H. L. Zhang
College of Chemistry and Chemical Engineering, Xiamen University

Transition metal oxides are being actively pursued as low-cost electrocatalysts for oxygen evolution reaction (OER) in many electrochemical energy devices. The OER activity is intrinsically determined by adsorption energetics of reaction intermediates and hence electronic structure of a catalyst. In this work, we report tuning of the electronic structure of NiO *via* Li doping ($Li_xNi_{1-x}O$) to enhance their OER activities. We have found that $Li_{0.5}Ni_{0.5}O$ has the highest OER activity, comparable to and exceeding those of mostly studied perovskite $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ and $LaNiO_3$. More importantly, a comprehensive combination of X-ray photoemission, X-ray absorption spectroscopy and density functional theory (DFT) was used to capture the electronic structure of $Li_xNi_{1-x}O$ with unprecedented accuracy. Our results reveal a strong hybridization between O 2p and Ni 3d, which is further enhanced with Li doping, leading to the remarkable enhancement of OER activity. A new unoccupied state develops at 0.5 eV above the Fermi level, and dominates at higher Li level. This unoccupied state acts as the acceptor to facilitate a fast electron transfer from OH^- to the catalyst. DFT calculations reveal that the improved OER activity originates from the facilitated adsorption of OH intermediates as Li doping. Our results represent an important advance towards the development of high-performance OER electrocatalysts.

A02-P22

Plasmon-Enhanced Photoelectrochemical Hydrogen Generation beyond Visible Region: The case of Au/CdSe Hybrid Nanorods from Core/shell to Nano-dumbbell

Hongzhi Wang*, Jia Liu, Jiatao Zhang
Beijing Institute of Technology

Plasmon enhancement contributed anisotropic metal/semiconductor hybrid photocatalyst requires not only the precise control of hetero-interface, but also the topology of its hetero-nanostructures, namely the intended configurations of photocatalytic semiconductor to anisotropic metal nanoparticle's plasmonic hot spots. In the case of Au nanorods (NRs), through water phase cation exchange strategy, the site-selective overgrowth of CdSe shell evolved from core/shell to nano-dumbbell have been realized successfully. By precise control of the selenization reaction, the core/shell Au/Ag NRs with controllable Ag shell could be conversed gradually from uniform core/shell to tip-preferred nano-dumbbell silver selenide, followed by the cation exchange enabled conversion to CdSe with expected crystallization and hetero-interface. Enabled by such, tip-preferred efficient photo-induced electron/hole separation and plasmon enhancement could be realized. Then photoelectrochemical (PEC) H_2 generation activity based on as-prepared Au/CdSe hetero-nanorods (H-NRs) formed photoanodes under Vis-NIR ($\lambda>700$ nm) illumination have been explored well. In particular, the nano-dumbbell Au/CdSe H-NRs have excellent performance with the faradic efficiency reach to 96% and excellent stability with constant photocurrent within 24 hours under Vis-NIR ($\lambda>700$ nm) light illumination.

A02-P23

Ligand Engineering on CdTe Quantum Dots in Perovskite Solar Cells for Suppressed Hysteresis

Jiawen Xiao*, Ma Sai, Shijie Yu, Chenxiao Zhou, Yujing Li, Qi Chen
Beijing Institute of Technology

Solar cells employing lead halide perovskites as light absorbers have been one hot topic in recent years due to their amazing device performance and commercialization potential. Yet, there exist challenges on the way to their practical use, including long-term stability, and J-V hysteresis. Herein, we demonstrate an improved contact between perovskite and hole transporting layer (HTL) by using CdTe quantum dots, wherein the capping ligands on quantum dots are systematically investigated. The devices with the CdTe quantum-dot-in-perovskite solids interlayer achieve a high efficiency (~19.3%, averaged), and more importantly, a significantly reduced hysteresis, which is superior to devices with CdTe QDs capped by other ligands (PbI_2, CH_3NH_3I, oleic acid). We attribute this superior device performance to the congeneric junction contact between perovskite and CdTe quantum-dot-in-perovskite layer. Furthermore, we reveal that the reduced hysteresis is partially contributed from faster hole extraction at the interface thanks to the high hole mobility in CdTe. These findings shed lights on the future design of quantum dots for perovskite optoelectronics in the perspective of ligand engineering.

A02-P24

Cross-sized and Cross-dimensional Self-assembly of Perovskite Nanocrystals on Flexible Substrate and Their Fluorescence Properties

Wenyi Huang*,Jiajia Liu,Jiatao Zhang
Beijing Key Laboratory of Construction-Tailorable Advanced Functional Materials and Green Applications, School of Materials Science & Engineering, Beijing Institute of Technology, Beijing, 100081, China

In recent years, perovskite nanocrystals have received great attention in the fabrication of highly efficient solar cells, light-emitting diodes (LEDs), and other optoelectronic devices, because their excellent photoelectric properties. Further advances will rely on structural variants that enable the formation of lower-dimensionality layered and three-dimensional (3D) perovskites with architectural innovations. In this work, the simple dip-coating method was used to obtained perovskite film and 3D assemblies of perovskite NCs were obtained through an attachment process. Original perovskite NCs had a rectangle or square morphology and the narrow symmetric fluorescence emission peak. The controllable self-assembly of the micron size cuboid-like 3D assembly had an apparent enhancement on peak (111) in the XRD diffraction pattern. The driving force of self-assembly is derived from the perovskite NC surface ligands which also served to maintain the independence of NCs. Such assembly perovskite film maintained original perovskite NCs fluorescent emission peak and narrow full width at the half-maximum (FWHM), which is of great importance for the application in future.

A02-P25

Naphtho[1,2-b:4,3-b']dithiophene-Based Hole Transporting Materials for High-performance Perovskite Solar Cells: Molecular Engineering and Opto-electronic Properties†

Binbin Cui*, Ning Yang
Beijing Institute of Technology

As a pump for extracting carriers from the absorber to the cathode, hole transporting material (HTM) has indispensable meanings to promote the power conversion efficiencies (PCE) of perovskite solar cells (PSCs). In this context, we present two simple HTMs using a 2,2'-(1,2-phenylene) bisthiophene or a naphtha[1,2-b:4,3-b']dithiophene as π-bridges to link two electron-donor (4',4''-dimethoxytriphenylamine): PBT and NDT. Their frontier molecular orbital energies match with that of perovskite well as is consistent to the DFT calculation results. The PCE measured under mimetic solar illumination (AM 1.5,V100 mW·cm-2) increases from 13.6% (PBT) to 18.8% (NDT), which surpass that of spiro-OMeTAD (18.1%) reference. The modified annulated core in NDT make it perform better in photovoltaic conversion ability than PBT. The reason for this is discussed from aspects of hole mobility, charge collection probability (Pc) and recombination kinetics.

A02-P26

Thiols Initialization and Solvents Coordination Enabled Novel Cation Exchange Strategy for Tailoring Composition and Property of Semiconductor Nanostructures

Bing Bai*, Meng Xu, J iatao Zhang
Beijing Key Laboratory of Construction-Tailorable Advanced Functional Materials and Green Applications, School of Materials Science & Engineering, Beijing Institute of Technology.

Considering the efficient and facile synthesis of versatile semi-conductor nanostructures, kinds of cation exchange ligands initialization and solvents coordination modulating the thermodynamics and kinetics of the cation exchange reaction were anticipated to synthesize complex semiconductor nanostructures with novel properties. In this work, various thoils initialization together with different solvent coordinations have been unprecedentedly used to explore new cation exchange strategy to synthesize complex semiconductor and metal@semiconductor nanocrystals. The detailed explorations by NMR characterizations and theoretical simulations have been carried out to investigate the novel reaction thermodynamics and kinetics. Furthermore, we have successfully synthesized high-quality *p-type* ZnS:Ag doped quantum dots (QDs) and the ZnS:Ag QDs emitted red fluorescence (luminescence peaks at 600 nm) via a ligand-solvent coordinate modulated cation exchange reaction, which have rarely been reported. The new-emerging metal@semiconductor nanocrystals and heterovalent doped QDs have been achieved efficiently.

A02-P27

From In doped Ag2S to AgInS2 NCs: synthesis and optical properties

Huishan Shang*,Jiatao Zhang
Beijing Key Laboratory of Construction-Tailorable Advanced Functional Materials and Green Applications， School of Materials Science & Engineering, Beijing Institute of Technology, Beijing, 100081, China

Monodisperse binary In^{3+} doped Ag_2S NCs and Ternary $AgInS_2$ NCs are reported by facile low temperature in-situ conversion of colloidal Ag_2S nanoparticles, where In^{3+} are inserted into the crystal lattice of Ag_2S NCs at low temperature following phase transition at high temperature. These doped Ag_2S NCs are explored further towards the position and intense of PL emission in different doping levels and the enhanced PL intensity compared with the low level doping is reported. Our results reveal that temperature may be a sensitive parameter to regulate the balance between cation reactivity and diffusion, according to the obtained In-doped Ag_2S NCs and $AgInS_2$ NC.

A02-P28

Photoelectronic Properties of Cu2O/Cu Semiconductor-Metal Hetero-nanocrystals: Enhancement from Cu metal nanocrystals

Muwei Ji*[1,2], Yao Hu[1], Ziyi Liu[1], Yiqing He[1], Chaozheng Li[3], Jiajia Liu[3], Jiatao Zhang[3], Li Bo[1], Caizhen Zhu[2], Jin Wang[1]
1. Tsinghua University, Graduate School at Shenzhen
2. College of Chemistry and Environment Engineering, Shenzhen University
3. Beijing Key Laboratory of Construction Tailorable Advanced Functional Materials and Green Applications, School of Materials Science and Engineering, Beijing Institute of Technology

Cu nanocrystal was considered unsuitable for electronic catalysis photocatalysis because of its low stability. However, Cu nanocrystals can be used as cocatalysis due to its enhancement of visual light aborption and excellent conductivity. Herein, we prepared Cu_2O/Cu hetero-nanocrytals via further reducing Cu_2O nanocrystals and transforming the Cu_2O nanocrystals into Cu_2O/Cu hetero-nanocrystals. The method for in-situ growth Cu on Cu_2O nanocrystals bring the photoelectronic properties enhancement of Cu_2O. The photocurrent of Cu_2O/Cu hetero-nancrystals was up to 190 $uA \cdot cm^{-2}$ which was obviously higher than that of Cu_2O nanocrystals under both UV and UV-vis irradiation. The circle voltammetry (CV) charaterization of Cu_2O/Cu hetero-nanocrystals on methanol oxiadation further confirmed the Cu enhacement of photoelectronic catalytic capacity under UV-vis irradiation. Cu_2O/Cu hetero-nanocrystals also performed at higher sensitivity than Cu_2O nanoparticles on ethanol gas sensing, which was also attributed to Cu metal enhancement.

A02-P29

Reduction of intrinsic defects in hybrid perovskite films via precursor purification

Deliang Zhang*, Bin-bin Cui
Beijing Institute of Technology

The crude MAI powder have been used by methylamine alcohol solution to purify, resulting in a substantial decrease of I2 in the final MAI precursor. This results in the enhancement of device performance, which is in part contributed from the facilitated charge transport within the device. The decrease in density of trap states is evidenced by the UV-vis absorption spectroscopy, TRPL, SCLC and the measurement of Urbach energy of each sample. This thus creates a sound correlation between the decrease of I2 in precursors and the decrease of trap density in the perovskite films, which finally improves the performance of photovoltaic cells. In addition, the proposed method provides an efficient and cost effective approach to fabricate high-quality perovskite absorbers with reduced trap density in a scalable manner, which paves the way toward of perovskite photovoltaics.In summary , a simple chemical process was developed in a scalable manner, to reduce trap states in perovskite absorbers from the very beginning. The obvious decrease of I2 in methylammonium iodide and the decrease of trap density in the resultant films were identified, which led to the power conversion efficiency (PCE) of perovskite solar cells (PSCs) increase from 16.5% to 18.5%.

A02-P30

The effect of W modification on structure stability and electrochemical performance of Ni-rich $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ cathode material

Ran Wang[*1], Jing Wang[1,2,3], Shi Chen[1,2,3], Yuefeng Su[1,2,3], Danhua Li[1], Ang Gao[1], Feng Wu[1,2,3]
1. Beijing Key Laboratory of Environmental Science and Engineering, School of Materials Science and Engineering, Beijing Institute of Technology, Beijing 100081, China
2. Collaborative Innovation Centre for Electric Vehicles in Beijing, Beijing, 100081, China
3. National Development Centre of High Technology Green Materials, Beijing, 100081, China

In recent years, nickel-rich layered oxide cathode materials have attracted worldwide interest due to its high energy density. However, it suffers rapid capacity fading and degradation of crystal structure during long charge/discharge processes especially at high cut-off voltage and elevated temperature. Herein, a facile method was carried out to increase the structural and interfacial stability of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ via W modification. The X-ray diffraction (XRD), transmission electron microscopy methods (TEM), and X-ray photoelectron spectroscopy (XPS) results demonstrated the successfully doping of W6+and the surface coating of fast ion conductor, Li_2WO_4. XPS analysis further analyzed the valence state change of nickel at the surface due to the incorporation of W^{6+}. From the electrochemical measurements, W1-NC electrode exhibited excellent cycling performance. Electrochemical impedance spectroscopy confirmed that the W^{6+} doping and Li_2WO_4 coating could improve the structural and interfacial stability, and hinder the impedance increase during cycling, which resulted in superior electrochemical performance.

A02-P31

Graphene quantum dots/Bi_2MoO_6 hybrid photocatalyst with efficient physical and chemical simultaneous co-catalysis for photocatalytic oxidation

Yuchen Hao*,Xiaoli Dong,Yu Wang,Nan Zheng
School of Light Industry and Chemical Engineering, Dalian Polytechnic University

1. Objectives

Over the past few years, the direct assembly of co-catalyst/modification materials into mesoporous photocatalysts has been considered a great challenge. Additionally, for photooxidation, the simultaneous achievement of fast charge separation, broad spectrum photocatalytic activity and higher carrier utilization efficiency (generating more active oxidizing groups) is quite necessary but has never been studied. To this end, for the first time, using sub-3 nm GQDs as co-catalyst, we have successfully achieved uniform modification for a mesoporous photocatalyst (mesoporous Bi2MoO6) using a novel electrostatic self-assembly method.

2. Methods

The sub-3 nm GQDs were prepared from graphene nanosheets by a modified chemical oxide method. And the hierarchical hollow mesoporous Bi2MoO6 were prepared by solvothermal method. The GQDs/M-Bi2MoO6 hybrid (GQDs–BM) was prepared through a surface charge modification method and a simple hydrothermal treatment.

3. Results

The sub-3 nm GQDs exhibit many unique physical and chemical properties, such as small size, electronic capture, up-conversion, and in particular, peroxidase-like activity. More importantly, we found that a certain amount of H2O2 was produced through a photoreduction effect during the photocatalytic process. Unfavorably, for bare Bi2MoO6, the continuously-accumulating H2O2 could not efficiently convert into OH by a one-photoelectron reduction, which results in the indirect waste of photo-excited electrons. Chemical co-catalysis of GQDs can efficiently enhance the photocatalytic activity of mesoporous Bi2MoO6 via photo-degradation activity for different target pollutants.

4. Conclusions

The photocatalyst were prepared by electrostatic self-assembly process, which can put the modification material in full contact with the mesoporous photocatalyst and achieve good dispersion within the mesoporous structure. After the GQDs were modified, the resulting mesoporous hybrid photocatalyst (GQDs-BM) exhibited excellent charge separation efficiency and broad spectrum photocatalytic activity from UV to NIR light. Moreover, GQDs could the chemical cocatalysis of GQDs could make the process (H2O2/?OH) more quick and efficient and moreover, did not need any additional photoelectrons, which means the effective enhancement of the utilization efficiency of photo-excited electrons (generating more ?OH). Additionally, for the as-prepared GQDs-BM, a sharp increase in photo-degradation activity for different target pollutants, further confirmed that the simultaneous physical and chemical co-catalysis of GQDs can efficiently enhance the photocatalytic activity of mesoporous Bi2MoO6.

A02-P32

Facile Synthesis of $NiCo_2$-$xFexO_4$ Nanotubes/Carbon Textiles Composites for High-performance Electrochemical Energy Storage Devices

Zhaohui Liu*, Longqiang Wang, Yufeng Cheng, Xiangyang Cheng, Bo Lin, Longfei Yue, Shougang Chen
Ocean University of China

To use advanced pseudo-capacitive electrode for improved energy density of supercapacitors has paid much attention recently. Herein, we develop a promising electrode architecture that containing carbon textiles uniformly covered with $NiCo_2$-$xFexO_4$ nanotubes, which are directly used as electrode materials in energy storages devices, through a simple and feasible two-step method and then a short period of post annealing treatment was adopted. The prepared $NiCo_2$-$xFexO_4$ nanotubes/carbon textiles composite electrode possesses a high specific capacitance of 2057 F g^{-1} when the discharging current is 1 A g^{-1}, and a superior long-life stability with 90.32% retention of specific capacitance after 3,000 cycles. The increased capacitive property is ascribed to the increased specific surface area, the vacancy formation and the unique nanotube structure.

A02-P33

A three-dimensional structure Si/Ni_3Si anode with high conductivity for Lithium-ion battery

Wurigumula Bao[*1], Jing Wang[1,2,3], Shi Chen[1,2,3], Feng Wu[1,2,3]
1. Beijing Institute of Technology
2. Collaborative Innovation Centre for Electric Vehicles in Beijing
3. National Development Centre of High Technology Green Materials

Despite the silicon-based anode suffers low conductivity and structural degradation during cycling, researchers are putting efforts on it due to its high capacity to meet the increasing demand of high energy density lithium-ion battery. The major capacity loss of silicon anode occurs in the initial few cycles and the coulombic efficiency is unsatisfying. Here we introduce a three-dimensional structure Si/Ni_3Si anode to tackle these problems. This unique designed electrode is achieved via plasma enhanced chemical vapor (PECVD), silicon nanoparticles were deposited onto three-dimensional nickel foam, which can function as 3D conductive networks. The networks provide abundant electrochemical activity sites and conductive transport paths. Besides, the electrode without additional binders or conductive agents can easily gain high energy density. The initial columbic efficiency is greatly improved by tuning the deposition time. With XRD characterization, a secondary phase of Ni_3Si is founded and serves as an inactive buffer matrix in the composite. High electrochemical performance is achieved with the 40 min deposition time. 694.9 mAh·g^{-1} specific capacity is delivered after the 50th cycles with 84.84% initial Columbic efficiency. This preferable performance is the result of the 3D conductive structure which enhanced physical and mechanical properties of the electrode.

A02-P34

Enhancing gas sensitivity and sensing mechanism at atomic and molecule level of WO_3 nanoparticles by hydrogenation

Qin Du*, Li Wang, Juan Yang, Junfang Liu, Yukun Yuan, Mengzhu Wang, Bin Liu, Xiao Zhang, Yan Ren, Hua Zhao, Heqin Yang
Shaanxi Normal University

In this work, we successfully developed a strategy for enhancing sensitivity of WO_3 nanoparticles by increasing density of the 5-fold coordinated unsaturated W atoms at the surface of WO_3 nanoparticles through hydrogenation. Responses of the hydrogenated WO_3 nanoparticles sensors towards alcohol, methanol and formaldehyde were found to be 2-3 times higher than that of the WO_3 nanoparticles without hydrogenation. We believed that the 5-fold coordinated W atoms function as the sensing reactive sites and elaborated the sensing reaction mechanism at atomic and molecule level. The 5-fold coordinated W atoms can absorb O_2 molecules, create conductive electrons and catalyze the sensing reaction between the absorbed O_2 with the detected gas. The concept of unsaturated 5-fold coordinated W atoms acting as the reaction active sites will be instructive for the in-depth understanding of sensing and other catalytic reaction as well as design of sensing materials and catalysts with outstanding performance. In addition, the hydrogenation activating surface strategy can be applied to increasing sensing and catalytic properties of other metallic oxides.

A02-P35

Hydrogenated TiO_2 nanosheet based flowerlike architectures : enhanced sensing performances and sensing mechanism

Junfang Liu*, Ye Wang, Miao Wang, Cuijin Pei, Meng Cui, Yukun Yuan, Guoping Han, Bin Liu, Hua Zhao, Heqing Yang,
Shengzhong Liu
Shaanxi normal university

TiO_2 nanosheet based flowerlike architectures with a surface area as high as 171 m^2 g^{-1} were prepared through a solvothermal method. The sensing performance of TiO_2 nanosheet based flowerlike architectures is enhanced by increasing density of surface unsaturated Ti atoms with dangling bonds through hydrogenation. We proposed a concept of the unsaturated Ti atoms serving as the sensing reaction active sites, and described in detail the sensing mechanism at the atomic and molecular level. The unsaturated Ti atoms not only generate non-contributing (free) electrons and adsorb oxygen molecules, but also catalyze the sensing reaction. In principle, the hydrogenation strategy may be used to improve sensing performances and catalytic activities of other metal oxides. The concept of the unsaturated metal Ti atoms serving as active sites can deepen understanding of the sensing and other catalytic reaction mechanisms, and provides a new insight to the design and fabrication of advanced sensing materials, catalysts and electronic devices.

A02-P36

Metal halide Perovskite Modified Garnet Electrolyte Enabled Enhanced-performance Solid State Li Metal Batteries

Jiafeng Wu*, Xinyue Li, Lang Liu, Wenjie Qu, Rui Luo, Lei Wei, Renjie Chen, Yujing Li, Qi Chen
Beijing Institute of Technology

Solid-electrolyte-based solid-state lithium batteries (SLBs) composed of garnet type have been investigated extensively, but the capacity of the garnet-based batteries is still not good enough to meet the requirements of commercialization of SLBs. Recently, metal-halide perovskites (MHP), including three-dimensional perovskite (3D-PVSK) and two-dimensional perovskite (2D-PVSK), are widely applied in researches on optoelectronic devices due to their excellent photoelectric properties. Recent studies have found that MHP can be embedded with small alkali ions (i.e. lithium and sodium ion). Therefore, 3D-PVSK and 2D-PVSK are utilized for the first time to deposit on the surface of garnet solid electrolyte ($Li_{6.75}La_3Zr_{1.75}Ta_{0.25}O_{12}$) through subsequence vapor-assisted and spin-coating process to improve the specific capacity of SLBs. We assemble MHP-modified and non-modified cells consisting of lithium anode, 3D-PVSK-modified, 2D-PVSK-modified and non-modified garnet and $LiFePO_4$ cathode. A significant increase in capacity of MHP-modified cell, the specific capacity of 160 mA h g-1 and 162 mA h g^{-1} for 3D-PVSK-modified and 2D-PVSK-modified cells after 50 cycling at 0.2C, is achieved with compared to that of non-modified counterpart (145 mA h g^{-1}), unambiguously illustrating the enhancement of lithium storage of SLBs with MHP modification. Our finding of increasing the capacity of SLBs via introducing MHP opens up a new path on the development of SLBs.

A02-P37

A Strategy in Fabricating New 2D Cesium Lead Halide Perovskite Material with Anionic Spacers

Yizhou Zhao*[1,2], Siyu Zhang[1], Xiuxiu Niu[1], Yue Lu[3], Zhu Cheng[1], Jiawen Xiao[1], Huachao Zai[1,2], Manling Sui[3], uanping Zhou[4], Yujing Li[1], Qi Chen[1]
1. Beijing Institute of Technology
2. China University of Petroleum
3. Beijing University of Technology
4. Peking University

The 2D halide perovskite have received enormous attention due to their unique photovoltaic and optoelectronic performances. Periodic spacers are used to inhibit the growth of 3D perovskite and fabricate 2D counterpart with layered structure, mostly based on organic/inorganic cations. So far, various organic/inorganic cationic molecules, including ammonium, amidinium, imidazolium, phosphonium, etc., have been used as periodic spacers to inhibit the formation of 3D perovskite structure by replacing the A-site ions (e.g. Cs^+, CH_3NH^{3+}, and $HC(NH)^{2+}$). In addition, Gemini-type bi-functional molecules with two ionic terminal groups serving as linkers between layers, such as diamine, amino acid, etc., have also been reported to obtain the layered 2D perovskite with extra functionalities. By introducing organic anions spacers between the inorganic sheets (e.g. pentanedioic acid (PDA) and hexanedioic acid (HDA) simultaneously), we have synthesized the leaf-shaped $(Cs_3Pb_2Br_5)$2(PDA-HDA) microplates with layered 2D structure. In contrast to the commonly studied 2D perovskite using cationic R-NH^{3+} as spacer, the -COO- anions are coordinated to Pb^{2+} forming an O-Pb-Br hybrid polyhedron. They also exhibit significant photoluminescence (PL) centered at 540 nm with a narrow emission peak of 17 nm. The synthesis of single crystals of Pb(PDA) and Pb(HDA) allows us to further clarify the crystal structure of $(Cs_3Pb_2Br_5)_2$(PDA-HDA) perovskite and its structural evolution mechanism. Moreover, the cooperative introduction of dicarboxylic acid pairs with appropriate lengths is thermodynamically favored for the 2D perovskite crystallization. This new layered structure demonstrates the possibility of forming the 2D perovskite by replacing the X-site ions, represents a new class of 2D hybrid perovskite, which also opens up a new approach to the growth of organic-inorganic hybrid 2D perovskite crystals.

A02-P38

Synthesis of p-Type Au@CdS by Cation Exchange Method and Its Utilization for Efficient photoelectrochemical Water Splitting

Rongrong Pan*, Jia Liu, Jiatao Zhang
School of materials science and engineering, Beijing institute of technology

Cu-doped Au@CdS semiconductor nanocrystal material was synthesized by cation exchange method for photoelectrochemical(PEC) water splitting. The resulting material was identified as p-type. In a systematic series of experiments, we used the n-type Au@CdS as the original material synthesized via cation exchange method, and the influence of the amount of copper doping on the p-type degree was studied. In order to study the type and density of charge carriers, we employed the open-circuit potential and Mott-Schotty measurements. Two methods showed the transition from n-type to p-type Au@CdS with increasing Cu-doped level. In addition, XPS and SEM-EDX also confirmed the Cu doping level. These results suggest substantial potential of p-type core-shell structure in PEC water splitting applications.

A02-P39

Pt-Ag porous alloy nanotube Rich in controlled Pt at the Surface with Enhanced Activity and Durability toward Oxygen Reduction

Erhuan Zhang*, Jia Liu, Jiatao Zhang
Beijing Key Laboratory of Construction-Tailorable Advanced Functional Materials and Green Applications, School of Materials Science & Engineering, Beijing Institute of Technology

Improving surface strains in heterogeneous catalyst and heteroatomic interactions in alloying soffers an effective strategy for the development of electrocatalysts with greatly enhanced activity. In this work, PtAg nanotubes (NTs) with connected single crystalline nanoparticles (NPs) is achieved by a simple galvanic replacement reaction using Ag nanowires (NWs) as sacrificial templates for its high and stable activity in the oxygen reduction reaction. The optimized PtAg NTs/C with a tunable structure and composition have high oxygen reduction reaction (ORR) activity that reach specific activities of 1.13 A cm^{-2} and mass activity of 0.688 A mg^{-1}Pt at 0.9 volts versus the reversible hydrogen electrode (RHE), which are 4.5 times and 4.3 times enhancements compared with a state-of-the-art commercial Pt/C catalyst (0.25 mA cm^{-2} and 0.16 A mg^{-1}Pt), respectively. Moreover, the porous PtAg-4 NTs have a much higher long-term durability than commercial Pt/C (20 %). In addition, we also investigated the enhancement mechanism.

A02-P40

X-ray scattering observation of two-dimensional interfacial colloidal crystallization

Longlong Wu*, Xiao Wang, Gang Chen
ShanghaiTech University

Colloids particles assembled into monolayer films at the air-water interface are central to a promising route to materials synthesis that combines considerable freedom of material choices with the opportunity to create highly ordered structures on the length scales from nano- to micrometers. Since the particles at the interface hold such a simple configuration that their interactions are supposed to be fully elucidated in the framework of classical electrostatics, the mysterious existence of attractive forces between these like-charged colloidal particles has puzzled the scientific community for decades.

Here, the in situ grazing-incidence small-angle X-ray scattering was used to study the dynamic self-assembling process of two-dimensional interfacial colloids at the Langmuir-Blodget (LB) trough. This approach allows simultaneous monitoring of the in-plane structure and ordering and the out-of-plane immersion depth variation.

Upon compression of the barriers on the LB trough, the system undergoes multiple metastable intermediate states before the stable hexagonal close-packed monolayer forms under van der Waals attraction. Remarkably, the immersion depth of colloidal particles is found to increase as the interparticle distance decreases. Numerical simulations demonstrate the interface around a colloid is deformed by the electrostatic force from its neighboring particles, which induces the long-range capillary attraction. These findings will give many useful directions to prepare the two-dimensional colloidal template over large scale.

A02-P41

Manipulation of facet orientation in hybrid perovskite polycrystalline films by cation cascade

Cheng Zhu[*1,2], Guanghaojie Zheng[2,3,4], Jingyuan Ma[4], Xiaonan Zhang[3,4], Gang Tang[1], Yihua Chen[2], Liang Li[1], Jinsong Hu[4], Jiawang Hong[1],Qi Chen[1], Xingyu Gao[3,4], Huanping Zhou[2]
1. Beijing institute of technology
2. Peking University
3. Shanghai Institute of Applied Physics Chinese Academy of Sciences
4. University of Chinese Academy of Sciences
5. Key Laboratory of Molecular Nanostructure and Nanotechnology
6. University of Science and Technology Beijing

Crystal orientations in multiple orders correlate to a wide range of properties of polycrystalline materials, and it is critical to manipulate these microstructural arrangements to enhance the corresponding device performance. Herein, we report a controllable approach to effectively manipulate the facet orientation (crystal stacking orientation) within the ABX_3 hybrid perovskites polycrystalline films by cation cascade doping at A site. Two-dimensional synchrotron radiation grazing incidence wide-angle X-ray scattering are employed to probe the crystal orientations in multiple orders in the mixed perovskites, clearly revealing a general pattern to guide crystal planes stacking upon extrinsic doping during film crystallization. Different from previous study that enables crystallization orientation or preferred growth over particular crystallographic planes, we revealed a controllable approach to effectively adjust the crystal stacking mode with respect to a certain crystallographic plane in polycrystalline perovskite thin films. Moreover, the preferred facet orientation introduced by cation cascade doping, is found to facilitate photo-carrier transport across the absorber and pertaining interface in the resultant PV device. This work further illustrates the feasibility to tailor the crystal stacking orientation of crystalline structure and consequent properties of hybrid perovskite materials in the intra-grain scale and provides an exemplary paradigm for further explorations that relate to the microstructures of hybrid perovskite materials, as well as wide-ranging optoelectronic polycrystalline semiconductors.

A02-P42

Heterovalent Sb^{3+}/Ag^{+} doping in CdS Quantum Dots with Efficient Tunable Luminescence: Cation Exchange Enabled Ternary Ag_3SbS_3 Nanocrystals conversion into doped binary CdS QDs

Qiumei Di*, Jiatao Zhang
Beijing Key Laboratory of Construction-Tailorable Advanced Functional Materials and Green Applications, School of Materials Science & Engineering, Beijing Institute of Technology, Beijing, 100081, China

Heterovalent doping in colloidal semiconductor quantum dots (CSQDs) could enhance their performance of optical and electronical properties. In this work, monodispersed pyrargyrite Ag_3SbS_3 QDs (5nm) were synthesized successfully the first time to our knowledge through in-situ reaction between Ag QDs and antimony mercaptide ($Sb(SCH_2COOC_8H_{17})_3$) of technical grade. The as prepared Ag3SbS3 QDs were chosen as the template to obtain Sb^{3+}, Ag^{+} co-doped CdS QDs via cation exchange with variable compositions. The as- synthesized doped CdS QDs exhibit efficient tunable defects photoluminescence from green (555 nm) to deep red (708nm). In addition, the co-doped CdS QDs show high absolute quantum yield (QY) up to 66.5% without any overcoating treatment. This kind of dopant emission with large stokes shift (0.83eV) could be stable for more than one year without any fading.

A02-P43

Inkjet-Printed Thermochromic Vanadium Dioxide Nanoparticle Films for Smart Windows

Haining Ji[*1,2], Dongqing Liu[2], Haifeng Cheng[2], Chaoyang Zhang[2]
1. School of Physics and Optoelectronic, Xiangtan University
2. Science and Technology on Advanced Ceramic Fibers and Composites Laboratory, National University of Defense Technology

Vanadium dioxide (VO_2) is a promising energy-saving material for next-generation smart windows that can respond to environmental temperature and modulate near infrared irradiation by changing from an infrared-transparent insulator state at low temperatures to an infrared-reflective metallic state at high temperatures, while maintaining its visible transmittance. It is commonly used in the films or coatings that function as smart windows. The usual methods for producing VO_2 films or coatings include magnetron sputtering, atomic layer deposition (ALD), chemical vapor deposition (CVD), physical vapor deposition (PVD), solution deposition methods and so on. While the vapor deposition techniques can provide high quality VO_2 films, solution deposition methods are more advantageous in cost-effectiveness and flexibility. But the preparation of a patterned smart windows by inexpensive methods still remains challenging until now. Inkjet printing is a powerful direct writing technique with the advantages of low cost, high resolution patterns, efficient use of materials, and applicability to various substrates, attracting escalating interests in fabricating optical and electrical devices. This study demonstrates a forefront and efficient inkjet printing technology for VO_2. First, a protocol was developed to generate stable and dispersible VO_2 nanoparticle inks for inkjet printing. The VO_2 films were then fabricated by printing VO_2 nanoparticle inks onto polyethylene terephthalate (PET) or float glass. The inkjet-printed VO_2 films exhibit a solar modulating ability (ΔTsol) of 15.31% with comparable visible transmittance. Its excellent performances have been further confirmed by smart window model. In addition, as a proof of concept the patterned VO2 films were also prepared via inkjet printing technology. We believe that our study makes a significant contribution to the state-of-the-art in a variety of applications of VO_2, which will better apply VO_2 nanoparticles to smart windows for green buildings and vehicles.

A02-P44

Dynamic Hosts for High-Performance Li-S Batteries Studied by Cryo-STEM and in Situ XRD

Xiaochen Liu*[1], Yao Yang[2], Héctor D Abruña[2], Fu-Sheng Ke[1]
1. College of Chemistry and Molecular Sciences, Wuhan University
2. Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University

Developing a high-performance sulfur host is central to the commercialization and general development of lithium sulfur batteries. Here, for the first time, we proposed a concept of dynamic hosts for lithium sulfur batteries and elucidated the mechanism through which TiS_2 acts as an example, using in situ X-ray diffraction (XRD) and cryogenic scanning transmission electron microscopy (Cryo-STEM). A TiS2-60S electrode delivered a reversible capacity of about 1120 and 886 mAh g^{-1} at 0.3 and 1.0 C, respectively, after 200 cycles, even a reversible capacity of 613 mAh g^{-1} at 1.0 C after 1000 cycles. Cryo-STEM and X-ray energy dispersive spectroscopy (XEDS) elemental mapping show that the TiS_2-S composite contains micrometer sized elemental sulfur particles with a well-defined morphology, and no evidence of sulfur infiltration into the TiS2 layers and covered on the surface of TiS_2. In situ XRD studies revealed the dynamic nature of TiS_2 during the discharge/charge process. TiS_2 exhibits reversible insertion/deinsertion of lithium ions to form $LixTiS_2$ ($0<x\leq1$). It is $LixTiS_2$ ($0<x\leq1$), rather than TiS_2, that plays a crucial role on the high capacity and superior stability of Li-S batteries. Furthermore, DFT calculations confirm the strong adsorption of polysulfides on $LixTiS_2$ ($0<x\leq1$), which can mitigate the polysulfide shuttling and improve the cycling performance. A fundamental understanding of the lithiation/delithiation dynamics of TiS_2 and TiS_2-S electrodes can serve as a guide for designing better sulfur host materials for Li-S batteries.

A02-P45

One-pot solvothermal synthesis of graphene/α-MnS nanocomposite for electrochemical capacitor electrodes

Xianfu Li*[1,2], Jianyu Zhou[1], Yingsong Yu[1], Kaixuan Zhou[1], Jianfeng Shen[2], Mingxin Ye[2]
1. Anhui Polytechnic University
2. Fudan University

Graphene/α-MnS nanocomposite was prepared by one-pot solvothermal reaction with graphene oxide (GO), $Na_2S_2O_3·5H_2O$ and $MnCl_2·4H_2O$. $Na_2S_2O_3·5H_2O$ plays an important role in being the reducing agent for GO and the sulfur source of α-MnS. All the X-ray diffraction (XRD) peaks of samples can be safely assigned to α-MnS (JCPDS card no. 65-0891) and graphene without noticeable impurity peaks. Scanning electron microscope (SEM) and Transmission electron microscope (TEM) observation identifies that α-MnS nanoparticles are uniformly distributed on the surfaces of graphene nanosheets. It is inferred that α-MnS nanoparticles on the surface of the graphene sheets can act as spacers to efficiently prevent the aggregation of the nanoparticles as well as the restacking of graphene sheets. The graphene/α-MnS nanocomposite exhibits a specific capacitance of 140.8 F g^{-1} at the voltage range of −0.55 to +0.55 V in a 6 M KOH aqueous solution electrolyte. Furthermore, the capacitance of the nanocomposite has no decrease of its initial values after 2000 cycles. The galvanostatic charge-discharge curve demonstrates the ideal capacitive behavior of graphene/α-MnS nanocomposite electrodes. The nanocomposite electrode exhibits a power density of 23.7 W kg^{-1} at a high current density, suggesting a good electrode material for supercapacitor.

A02-P46

Grain Boundary “Patches” by in situ Conversion to Enhance Perovskite Solar Cells Stability

Lang Liu*[1], Sheng Huang[1], Yue Lu[2], Pengfei Liu[1], Yizhou Zhao[1], Congbo Shi[1], Siyu Zhang[1], Jiafeng Wu[1], Haizheng Zhong[1], Manling Sui[2], Huanping Zhou[3], Haibo Jin[1], Yujing Li[1], Qi Chen[1,4]
1. Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Materials Science & Engineering, Beijing Institute of Technology, Beijing 100081, China
2. Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing 100124, China
3. Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, China
4. Advanced Research Institute for Multidisciplinary Science, Beijing Institute of Technology, Beijing 100081, China

The power conversion efficiency of organic-inorganic hybrid perovskite solar cells increases rapidly, but the device stability remains a big challenge. Previous studies show the grain boundary (GB) can facilitate ion migration and initiate the device degradation. Herein, the methimazole (MMI) is employed for the first time to construct the surface “patch” by in situ converting residual PbI2 at GBs. The resultant MMI-PbI2 complex can effectively suppress the ion migration and inhibit the diffusion of metal electrodes. The origin of the surface “patch” effect and their working mechanisms are investigated experimentally and theoretically at the microscopic level. It hence demonstrates a simple and effective method to prolong the device stability in the context of GB engineering, which could be extensively applied to perovskite-based optoelectronics.

Keywords: perovskite solar cells, patch, grain boundary engineering, stability, methimazole

A02-P47

Direct Anodic Exfoliation of Graphite onto High-density Aligned Graphene for Large Capacity Supercapacitors

Liangsheng Hu*, Kwok-Yin Wong
The Hong Kong Polytechnic University

Vertically oriented graphene nanosheets (VOGNs) fabricated on conductive substrates with a large amount of edge planes and

the open channels are ideal for electrochemical double-layer (EDL) capacitor electrodes. However, preparation of such a structure with a high-density of graphene nanosheets is challenging. Herein, a facile, environment-friendly, and economical technique to prepare high-quality VOGNs directly on highly conductive graphite plates with a high mass loading is described. The VOGNs are obtained by electrochemical anodization of graphite. A large amount of aligned reduced graphene oxide (rGO) is produced and adheres strongly to the graphite substrate (G@rGO) followed by reduction. The symmetrical supercapacitors composed of the G@rGO electrodes exhibit a high volumetric capacitance of 3.9 F cm^{-3} and energy density of 0.66 Wh L^{-1} (based on the volume of the whole electrode) at a current density of 7.5 mA cm^{-3} in 6 M KOH. The rate performance and long-term cycling stability are thus very good. The outstanding capacitive performance can be attributed to the unique structure of the G@rGO electrode which facilitates transportation of ions between the electrolyte and graphene surface, minimizes the distributive nature of charge storage, expedites the formation of EDL, and enhances the electrochemical utilization of graphene and stability by avoiding restacking and aggregation of graphene nanosheets.

Keywords: Aligned graphene, Supercapacitor, Electrochemical exfoliation, Energy storage

A02-P48

Mn7C3 confined in the mesoporous carbon spere for high rate Lithium-sulfur batteries.

Xiaoqiang Liang*[1,2], Xiong Pu[1,2]

1.Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences

2.University of Chinese Academy of Science, Academy of nanoscience and nanotechnology

Lithium−sulfur batteries (Li−S) have attracted more and more attention due to the particularly high energy density for advanced energy storage system.Herein, we have synthesized a novel composite eletrode materials,Mn_7C_3@MC. Firstly,a novel type of mesoporous carbon sphere(MC) have been synthesized via hydrothermal treatment by using resol as the carbon source and triblock copolymer Pluronic F127 as the template. Post hydrothermal treatment,the sample was soaked in $KMnO_4$ solution.Then sulfur was encapsulated in the Mn_7C_3@MC materials by a simple thermal treatment.Homogeneous porous distribution rising from inside and outside of MC provide an effective conductive network for sulfir and polysulfides during cycling.In addition,crystalline Mn_7C_3 contributes to capacity improvment.The composite materials exhibit high reversible capacity,good capacity retention high rate electrochemical characterization when used as cathode in rechargeable lithium–sulfur batteries.The resulting S@Mn_7C_3@MC electrode delivers a discharge capacity of 1035 mAh/g at 0.25C,524.2mAh/g at 5C. Moreover,69.2% and 70.7% capacity retention at 0.5C and 1C respectively.

Keywords: Lithium−sulfur batteries, Mn7C3, MC,high rate, capacity

A02-P49

Controllable Preparation of Tungsten / Tungsten Carbide Nanowires Using Carbon Nanotubes as Templates

Xiaona Ren*, Min Xia, Qing-Zhi Yan, Chang-Chun Ge, Xian-Ran Xing

University of Science and Technology Beijing

Since Tungsten (W) features with excellent properties like high melting point, density, harness and outstanding wear-resisting, W and W-based materials are important materials and widely used in fields like national defense, aerospace, electronic information, energy, metallurgy and nuclear. In particular, the nano-sized W or W-based materials are more important and widely applied. For example, W-nanowires have been used as strengthen phase for plastic composites, bullet, shot, radiation shields, or used as substitute for uranium along with iron and steel matrix. What's more, W-nanowire has been used as metal gate, Li-ion battery catalyst, pH sensitive electrodes, hydrogen sensor, electron emission sources, template for nanodots, etc.. On the other side, as a kind of important W-based material, tungsten carbide not only has been widely used as cemented carbide but also is considered as green catalyst for diverse electron-transfer reactions, as it possesses platinum-like behavior, e.g. tungsten carbide has been widely studied as catalyst for isomerization reactions, fuel cells, hydrogenolysis, hydrogen evolution and catalytic oxidation or used in biology as artificial enzymes.

Whereas, a preparation method of W or W-based nano-materials has seldom been founded, which could realize preparation of large-scale, morphology controllable and none catalyst involved. Here we proposed a novel and controllable preparation method that applies mesoporous carbon nanotubes (mCNTs) as templates. By utilizing the tubular structure of mCNT and capillarity of mesoporous in the side wall of mCNT, we successfully prepared W nanowires and di-tungsten carbide (W2C, an unstable phase of

tungsten carbide) nanowires. To be specifically, lab prepared mCNTs were hydrophilia functionalized and then dipped into specific aqueous solution of ammonium metatungstate (AMT), AMT nanorods in mCNTs could be obtained after filtration and drying. The most important step is the reduction of AMT nanorods in mCNTs by H_2. Large scale, shape controllable and none catalyst W-nanowires could be prepared with optimized reduction parameters. And then the as-obtained W-nanowires could be converted to W2C nanowires simply by means of heat treatment. The as-gained W-nanowires and W2C nanowires features with diameter of circa 50nm and length varies with the length of mCNTs.

Keywords: tungsten nanowire, tungsten carbide, mesoporous carbon nanotubes, wet chemical, template

A02-P50

One-pot synthesis of Pt72Ru28 Porous Nanoalloy Assembled with Sub-4.0 nm Particles for Methanol Oxidation

Fengling Zhao*, Wei yue Zhao, Qiang Yuan
Guizhou University

The main challenges to the direct methanol fuel cells are the activity and durability of electrocatalysts. To alleviate such issues, a recently proposed strategy introduces an exotic element to form Pt-based alloy nanostructures. This study reports a green route to prepare porous flowerlike $Pt_{72}Ru_{28}$ nanoalloys assembled with sub-4.0 nm particles. The peak current density and mass activity on these as-synthesized porous flowerlike $Pt_{72}Ru_{28}$ nanoalloys can be increased to 10.98 mA cm^{-2} and 1.70 A $mg^{-1}{}_{Pt}$ for methanol oxidation in acidic medium. They are respectively 4.19/3.54, 4.27/5.0, and 5.74/1.73 times those on the commercial Pt black, $Pt_{50}Ru_{50}$ black,and Pt_{50} Ru_{50} /C. These porous flowerlike $Pt_{72}Ru_{28}$ nanoalloys have a much higher long-term durability than commercial Pt black, $Pt_{50}Ru_{50}$ black, and $Pt_{50}Ru_{50}$ /C. More significantly, the porous $Pt_{72}Ru_{28}$ bimetallic nanoalloys have long-term solvent durability after immersion in water for 16 months.The peak current density and mass activity on porous $Pt_{72}Ru_{28}$ nanoalloys are still 7.76 mA cm^{-2} and 1.2 A $mg^{-1}{}_{Pt}$. These experimental results show an effective approach to the development of PtRu nanoalloys as electrocatalysts with substantially enhanced activity and durability for direct methanol fuel cells.

Keywords: PtRu nanoalloy, porous structure, methanol oxidation, fuel cells.

A02-P51

Enhanced upconversion based on the ultrahigh local field enhancement in a multilayered UCNPs-metamaterial composite system

Shiping Zhan*[1], Xiaofeng Wu[1], Chao Tan[1], Jian Xiong[2], Shigang Hu[1], Junshan Hu[1], Shaobin Wu[1], Yongyi Gao[1], Yunxin Liu[1]
1. Hunan University of Science and Techology
2. Guilin University of Electronic Technology

In this paper, we reported a multilayer metamaterial system with ultrahigh absorption, consisting of silver nanoring, upconversion nanoparticles(UCNPs) and silver film, which can dramatically enhance the upconversion emission. A simplified theoretical expression of the upconversion enhancement factor(EF_{upc}) was derived, and the structure parameter and the local field-UCNPs coupling were considered for the EF_{upc} analysis. It was found that the bottom silver film was crucial for the tremendous upconversion enhancement since it gave rise to a pronounced absorption peak and resulted in a strong field confinement of the 980 nm excitation light. Comparing with the nanodisk, the nanoring performed better in enhancing the upconversion, and an enhancement factor of $\sim 3.2 \times 10^4$ was achieved based on the numerical and theoretical analysis. This metamaterial system provided a novel approach in enhancing upconversion, and the research findings could be helpful to the design of biosensor and photovoltaic devices.

Keywords: Surface plasmon, Upconversion nanoparticle, Emission enhancement, Perfect absorption, Metamaterial

A02-P52

Enhanced gas separation performance of Ionic Liquid Nanoconfined in MoS2 nanochannels

Danke Chen*, Xinsheng Peng
State Key Laboratory of Silicon Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou, China

Aims: Recently, 2D materials constructed membranes have shown promising potential for separation processes. In order to improve the gas separation performance of MoS_2-based membrane, filling another material with good gas separation performance into the 2D channels of MoS_2 membrane is a promising way. In present work, 1-butyl-3-methyl imidazolium tetrafluoroborate ([BMIM][BF_4]) was chosen to be confined into the 2D channels of MoS_2 laminated membranes for gas separation, since

[BMIM][BF_4] is an economical IL and has high solubility of CO_2.

Methods: MoS_2 nanosheets were exfoliated by Liquid Exfoliation with n-butyl lithium in an Ar-filled glove box. MoS_2 membrane was prepared by vacuum filtrating 3~5 ml diluted MoS_2 nanosheets dispersion (0.29 mg/ml) on an AAO substrate. 0.2~1 ml [BMIM][BF_4] was dropped on the obtained MoS_2 membrane. After 12~72 h, [BMIM][BF_4] would enter into MoS_2 two-dimensional channels via strong capillary force and finally confined in the channels to form MoS_2 supported ionic liquid membranes (MoS_2 SILM). The excess ionic liquid was wiped off with filter paper.

The gas permeation measurement of MoS_2 membrane and MoS_2 SILMs was determined by a constant-pressure variable volume method. The upstream pressure was 0.16 MPa, while the downstream pressure was 0.10 MPa (atmosphere pressure). The gas measurements for gas molecules of different kinetic diameters (e.g., H_2 (0.289 nm), N_2 (0.364 nm), CH_4 (0.384 nm) and CO_2 (0.330 nm)) were tested at room temperature. Gas flow rate was detected with a bubble flow-meter with effective membrane area being 2.99 cm^2.

Results: A series of MoS_2 SILMs are fabricated through dropping a certain volume of [BMIM][BF_4] on the surface of the as-prepared MoS_2 membranes, while [BMIM][BF_4] is uniformly filled between the MoS_2 layers without conspicuous voids.Compared to the corresponding bulk [BMIM][BF_4], confining ILs in the channels of MoS_2 leads to an increment of 5.5 °C in freezing point, which ensures the stability of [BMIM][BF_4] in MoS_2 SILMs. MoS_2 SILMs also shows apparent vibration bands shift of FTIR spectra due to the interactions between ILs and the channel walls, which partly reveals the nanoconfined [BMIM][BF_4] has uncommon physicochemical properties.

The resulted MoS_2 SILM exhibits superb CO_2 separation performance with high CO_2 permeance (47.88 GPU) and fantastic selectivity of CO_2/N_2 (131.42), CO_2/CH_4 (43.52) and CO_2/H_2 (14.95), which is much better than neat [BMIM][BF_4] and [BMIM][BF4]-based membranes. Besides, the as-prepared MoS_2 SILM shows nice durability for seven days. The excellent performance of the prepared MoS_2 SILMs mainly results from the effects of nanoconfined ILs.

Conclusions: MoS_2 SILMs with high CO_2 permeability and selectivity are fabricated by confining [BMIM][BF_4] into the 2D channels of MoS_2 laminated membranes. The nanoconfinement of ILs results in high CO_2 permeance and superior selectivity for CO_2/N_2, CO_2/CH_4 and CO_2/H_2 pairs of MoS_2 SILMs with nice durability far more than pure MoS_2 membrane, neat [BMIM][BF_4] and other [BMIM][BF_4]-based membranes. Confining ILs into 2D channels of 2D materials via infiltration process may open a new avenue for highly efficient membrane for separating CO_2 from other light gases.

Keywords: nanoconfined ionic liquid, MoS2 nanosheets, CO2 separation, two-dimensional channels

A02-P53

Ionic liquid selectively facilitates CO_2 transport through graphene oxide membrane

Wen Ying*, Xinsheng Peng
School of Materials Science and Engineering, Zhejiang University

Aims: Separating CO_2 from other gases, such as H_2, N_2 and CH_4, has economic benefits. Membrane separation is a potential technic for CO_2 separation, while trade-off between selectivity and permeance is a challenge. We make this work to fabricate a membrane with both high permeance and high selectivity.

Methods: We immobilized 1-butyl-3-methylimidazolium tetrafluoroborate ([BMIM][BF_4]), an inexpensive room temperature ionic liquid with a high CO_2 solubility and low H_2, CH_4 and N_2 solubilities, into the 2D nanochannels of laminated graphene oxide (GO) membranes by dispersing GO into ionic liquid and filtering on the AAO membrane. GO was prepared by modified Hummer's method. The resultant membrane was mainly characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), solid-state nuclear magnetic resonance (SSNMR) and bubble flow meter.

Results: Ionic liquid is uniformly dispersed and nanoconfined into the nanochannels, which was confirmed by SEM and SSNMR. The nanoconfinement causes the [BMIM][BF_4] cations and anions to stratify. The resultant GO-SILMs facilitate CO_2 transportation by the layered anions with a permeance of 68.5 GPU, and extremely high CO_2/H_2, CO_2/CH_4 and CO_2/N_2 selectivities, that are 24, 234, and 382, respectively, which are up to 7 times greater than those of GO-based membranes and superior to that of most state-of-the-art membranes. Additionally, the resultant membrane has a high-temperature resistance, long-term durability and high-pressure stability.

Conclusions: A high-performance CO_2-philic membrane, GO-SILM, was developed by nanoconfining [BMIM][BF_4] into the 2D nanochannels of a GO membrane. The nanoconfined [BMIM][BF_4] significantly facilitates the transportation of CO_2 and improves the selectivity for CO_2 over other gases. The high-temperature resistance, long-term durability and high-pressure stability of GO-SILMs show the great potential of CO_2 separation and competitive to polymer-supported IL membranes.

Keywords: nanoconfinement; graphene oxide-supported ionic liquid membranes; gas separation;

A02-P54

Fe_2N encapsulated in N-doped porous carbon derived from MOFs as synergistic catalyst for ORR

Xiaoxiao Huang*, Yanglong Hou
Peking University

The oxygen reduction reaction (ORR) is one key step in fuel cells and metal air batteries. However, the cathodic catalyst Pt suffers from high cost, severe scarcity, and low stability. Over the past few years, transition metal-nitrogen/carbon (M-N/C) based catalysts as alternatives for ORR have been intensively explored.

Pyrolyzed MOFs materials have been explored as efficient ORR catalysts with large surface area, abundant pore structures and exposed active sites. However, the traditional MOFs-derived ORR catalysts illustrate ORR performance gap with benchmark Pt/C in ORR performance for: 1) limited active sites caused by the specific coordination of metal ions and ligands in MOFs precursors; 2) insufficient exposure of active sites for the agglomeration of NPs in high-temperature pyrolysis process.

Herein, we developed a Fe_2N nanoparticles (NPs) incorporated in N doped porous carbon (Fe_2N@NPC) derived from MOFs as a highly active ORR catalyst, which can well address the afore-mentioned drawbacks. The Fe_2N@NPC can be synthesized by a two-step annealing process, in which the second annealing step can produce uniform distribution of NPs at lower temperature. What is more, the various addition of metal precursors can produce diverse amounts and varieties of active sites. The resultant Fe_2N@NPC-500 catalysts show comparable onset potential and half-wave potential to commercial Pt/C catalyst, as well as better stability and methanol tolerance. The outstanding ORR performance of Fe_2N@NPC-500 is due to the large amount of the ORR active Fe-N/C bonding formed by Fe_2N nanoparticles and N doped carbon. Besides, the porous N doped carbon facilitates the mass transport of O_2 and electrolyte, as well as improves the conductivity. It is also worth noting that the synthesis routine also provides possibility for producing other non-precious metal catalysts for ORR, presenting a new strategy for substituting Pt catalysts in fuel cells.

A02-P55

Stable p-type ZnO Nanowires for photoelectrochemical and photocatalytic water splitting

Chang Cao*, Shiwei Lin
Hainan University, State Key Laboratory of Marine Resource Utilization in South China Sea

The high quality of ZnO nanowire arrays determines their high performance of the photoelectrochemical (PEC) water splitting properties. ZnO is considered as a promising material for optoelectronic devices. However, the development of ZnO-based nano-electronic devices has been limited owing to the difficulty of obtaining stable p-type ZnO. V group elements are generally used in doping ZnO to get p-type conductivity, and antimony (Sb) has been shown to be the promising candidate for preparing p-type ZnO.

In this work, we adopted two-step method to prepare p-type Sb-doped ZnO nanowires. The uniform ZnO seed film was obtained by atomic layer deposition (ALD). And then a hydrothermal method was conducted to control Sb doping into ZnO nanowires to achieve p-type ZnO.

The structural studies showed that the Sb:ZnO nanowires had high crystallinity with c-axis orientation. The UV-vis results demonstrated that Sb doping into ZnO could significantly improve the light absorption. Mott-Schottky were further measured to prove the typical characteristics of p-type semiconductors of the prepared Sb:ZnO. The cathodic photocurrent density of p-0.2 reached -0.28 mA/cm^2 (0 V vs RHE), which is 2.5 times higher than the pure n-type ZnO, which reflected more efficient charge transfer and separation Sb:ZnO. The reasons for the improvements of PEC performance would be the fewer defects states and high carrier density due to the doping of Sb elements. Further work about the effect of thermal treatment on the photocurrent density was also discussed.

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Keywords: p-type; ZnO; photoelectrochemical

A02-P56

Free-Standing N-doped Carbon Nanofibers/Carbon Nanotubes Hybrid Film for Flexible, Robust Half and Full Lithium-ion Batteries

Ling Huang*[1,2], Qun Guan[1,2], Jianli Cheng[1,2], Bin Wang[1,2]
1. Institute of Chemical Materials, China Academy of Engineering Physics
2. Sichuan R&D Center of New Materials

With the flexible electronics prevailing, the energy storage devices with outstanding flexibility, high power and energy density, as well as long cycle-life, are attracted many people. Recently, we masterly integrated carbon nanofibers(CNFs) and carbon nanotubes(CNTs) to prepare free-standing N-doped carbon films with hierarchical structure of CNFs/CNTs hybrids via a simple electrospinning process. This interconnected CNFs/CNTs hybrid film show high conductivity and excellent flexibility. When the CNFs/CNTs hybrid film used as a free-standing and binder-free anode material, they show a highly reversible specific capacity, excellent cycling stability and rate performance (maintained over 1099.5 mAh g^{-1} at a current density of 0.05 A g^{-1} after 100cycles). The remarkable electrochemical performance mainly lied in the unique hierarchical structures of nanofibers and nanotube hybrids of N-doped carbon hybrid film. What's more, this hybrid film used in the lithium-ion battery could withstand the bending at different angles and release a stable discharge capacity of 463.6 mAh g^{-1} after 60 cycles at various bending positions (0°, 45°, 90°, and 180°) at a current density of 0.5 A g^{-1}. Meanwhile, flexible full Li-ion battery based on CNFs/CNTs// $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ could also display excellent flexibility and be able to light up a “C” pattern lighting emitting diodes (LEDs) in the flat, 90°, 180°, and 360° bending positions, respectively, being a potential candidate for flexible energy storage devices.

Keywords: flexible; N-doped carbon nanofibers; carbon nanotube; anode

A02-P57

High-throughput preparation and characterization of perovskite microflakes based on microdroplet array

Huigang Du*
Shanghai University

In early 2015, Protesescu et al.[1] reported pioneering work on all-inorganic cesium lead halide ($CsPbX_3$, X = Cl, Br, and I) light-emitting nanocrystals. Immediately after their report, there was an explosion of research activity on all-inorganic metal halide perovskite nanostructures (IHPNs) motivated by their superior optical properties and the low cost of the synthetic methods. Besides, it overcomes the disadvantages of organic-inorganic halide perovskites that are extremely sensitive to the moisture, oxygen, and heat[2]. Due to its superior performance, striking development of IHPNs has been witnessed in terms of fabrication strategies, optical characterization, and optoelectronic applications with the effort of the researchers. However, there is less research on the growth process of the perovskite during these processing due to its fast process. We developed a facile method to in situ analyst from micro-droplets.

Zheng et al.[3]reported a low-cost and high-compatibility one-step liquid-phase synthesis method for synthesizing high-purity $CsPbBr_3$ micro-/nanoflake single crystals. Based on this work, we find it is possible to control the crystallization of perovskite in the microdroplet with the balance of the evaporation and concentration. We form thousands of droplets of DMF-$CsPbBr_3$ solution precursor on the prepatterned surface[4]with a controllable sliding method for fabricating millions of isolated femto- to nanoliter-sized droplets with defined volume, geometry and position to realize perovskite growth position and crystal morphology on surface, achieving higher-throughput generation compared to other methods.At the effect of evaporation induced self-assembly, highly uniform micro-/nanoflake $CsPbBr_3$ perovskite crystal arrays. It is a important applications in photoelectric detector, luminescent device and so on.

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Keywords: Perovskite*; hydrophilic/hydrophobic patterning;* crystallization; *high-throughput*.

A02-P58

Boosting the Deep Discharging/Charging Lithium Storage Performances of Li3VO4 through Double-Carbon Decoration

Huancheng Liu*, Ping Hu, Qiang Yu, Zhenhui Liu, Ting Zhu, Wen Luo, Liang Zhou, Liqiang Mai
Wuhan University of Technology

With high theoretical capacity, good ionic conductivity, and suitable working plateaus, Li_3VO_4 has emerged as an eye-catching intercalation anode material for lithium storage. However, the Li_3VO_4 suffers from poor electrical conductivity and 20% volume variation under deep discharging/charging conditions. Herein, we present a "double-carbon decoration" strategy to tackle both issues. Deflated balloon-like Li_3VO_4/C/rGO (LVO/C/rGO) microspheres with continuous electron transport pathways and sufficient free space for volume change accommodation are fabricated through a facile spray drying method. Under deep discharging/charging conditions (0.02 – 3.0 V), the LVO/C/rGO achieves a high intercalation capacity of 591 mAh g^{-1}. With high capacity and outstanding stability, the LVO/C/rGO outperforms other intercalation anode materials (such as graphite, $Li_4Ti_5O_{12}$, and TiO_2). *In-situ* XRD measurement reveals that the lithium storage is realized through both solid-solution reaction and two-phase reaction mechanisms. A LVO/C/rGO//$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ lithium-ion full cell is also assembled. In such full cell, the LVO/C/rGO also demonstrates high specific capacity and excellent cycling stability.

Keywords: Li_3VO_4, spray drying, intercalation anode, lithium-ion battery, double-carbon decoration

A02-P59

Composition-driven shape evolution to Cu-rich PtCu octahedral alloy nanocrystals as superior bifunctional catalysts for fuel cell

Fang Yang*, Chaozhong Li, Qiang Yuan
Guizhou University

Synergetic effect between Pt and cheap metal, downshift of the d-band center of Pt and the shape can boost the catalytic performance of Pt-based nanocrystals. Therefore, tailoring the shape and composition within the nanoscale is the key to designing robust electrocatalyst in electrochemical energy conversion. Here, Cu-rich PtCu octahedral alloys achieved by composition-driven shape evolution route have been used as outstanding bifunctional electrocatalysts for both methanol oxidation (MOR) and oxygen reduction reaction (ORR) in acid medium. When benchmarks against commercial Pt black or Pt/C, for MOR, the specific activity/mass activity on $Pt_{34.5}Cu_{65.5}$ octahedrons is 4.74/7.53 times higher than that on commercial Pt black; for ORR, the specific activity/ mass activity on $Pt_{34.5}Cu_{65.5}$ octahedrons is 7.7/4.2 times higher than that on commercial Pt/C. After current-time test for 3600s, the remaining mass activity on $Pt_{34.5}Cu_{65.5}$ octahedrons is 35.5 times higher than that on commercial Pt black for MOR. And undergoing 5000 cycles for ORR, the remaining mass activity on $Pt_{34.5}Cu_{65.5}$ octahedrons is 4.2 times higher than that on commercial Pt/C.

Keywords: PtCu alloy, shape evolution, methanol oxidation, oxygen reduction reaction,fuel cell

A02-P60

Controlled Cation Exchange Reaction between Cu^{2+} and Bi_2Te_3 nanoplate: Controlled Synthesis, Characterization and Mechanism

Xiangyun Bai*, Ning Su, Shuai Guo, Yuxiong Chen, Jin Wang, Muwei Ji, Bo Li
Graduate School at Shenzhen, Tsinghua University

Bismuth Telluride (Bi_2Te_3) has been applied to thermoelectric generation and refrigeration due to its great thermoelectric properties near room temperature. It has been proved that 2D ultrathin nanoplates has better thermoelectric performance, which can be further improved by ions doping. Doping is an important technology for construct nanocrystals and allows controlling the crystal structure of Bi_2Te_3 nanoplate to enhance their Seebeck coefficient, conductivity, and thermal conductivity.

In our study, Bi_2Te_3 nanoplates were prepared by solvothermal synthesis of $BiCl_3$ and K_2TeO_4 in KOH solution and polyvinyl pyrrolidone (PVP) was used as surfactant in the reaction. Followed by, Cu^{2+} is introduced into Bi_2Te_3 nanoplates via cation exchange reaction in aqueous solution. Successful doping is confirmed by high resolution transmission electron microscopy (HRTEM) and X-ray photoelectron spectra (XPS) characterizations. Atom-force microscopy (AFM) and scanning electron microscopy (SEM) results shows that, with increasing dopant level, holes produce and grow in the center of the nanoplates resulting in formation of hexagonal nanorings at high doping level.

Based on above observations, we proposed the mechanism for cation exchange reaction between Cu^{2+} and Bi_2Te_3 nanoplates: Cu^{2+} replacing preferred sublattice sites of Bi^{3+} and Cu^{2+} diffusion leads to the gradual change of the crystal structure, then the collapse of the central part of the Te^{2-} framework and thereby nanorings form with the origin shape of Bi_2Te_3 nanoplates.

A02-P61

Monodispersed sub-5.0 nm PtCu nanoalloys：composition-tunable synthesis and their applications for oxygen reduction reaction and ethanol oxidation reaction

Tengyue Ma*, Taiyang Liu, Qiang Yuan
Guizhou University

The development of effective electrocatalysts with enhanced activity and stability for both the anode and the cathode reaction in fuel cells still remains a challenge. Here, we report a one-pot route to prepare monodispersed, uniform sub-5.0 nm PtCu alloy polyhedra with a narrow size distribution. These PtCu alloy polyhedral exhibit enhanced electrocatalytic activity for both cathode and anode reactions as compared to the commercial Pt/C catalyst under alkaline conditions. The specific activity and mass activity on $Pt_{68}Cu_{32}$ nanoalloys are 15 and 2.8 times that on Pt/C catalyst toward oxygen reduction reaction (ORR), respectively. And the peak current density and mass activity on $Pt_{68}Cu_{32}$ nanoalloys are 11.8 and 2.12 times that on Pt/C catalyst toward ethanol oxidation reaction (EOR), respectively. Furthermore, the as-synthesized $Pt_{68}Cu_{32}$ nanoalloys have much higher stability than commercial Pt/C black for both ORR and EOR. These experimental results show an effective approach to the development of monodispersed, sub-5.0 nm PtCu nanoalloys as bifunctional electrocatalysts for both the cathode and the anode reaction in fuel cells.

Keywords: monodisperse; PtCu nanoalloys; oxygen reduction reaction; ethanol oxidation reaction; fuel cells

A02-P62

Low temperature derived atomic cobalt on N-doped graphene as an efficient electrocatalyst for the oxygen reduction reaction and Zn-air batterie

Haoyun Liu*
WuHan University of Technology

The development of low-cost metal-based electrocatalysts for oxygen reduction reaction holds the decisive key to new-generation fuel cells and metal-air batteries. Co-N-C catalysts have gained increasing attention for substituting precious catalysts. Herein, we made a highly reactive and stable atomic Co/N-doped graphene catalyst with Co loading up to 2.89 at%. The catalyst showed excellent electrochemical performance. In 0.1 M KOH, CoNG-350 exhibits a cathodic potential about 0.9 V vs RHE, a much higher limiting current density of 5.60 mA cm^{-2}, low peroxide yield of <9% and great stability, which outperformed most nonprecious metal-based electrocatalysts reported to date. Specifically, when the catalyst was used as the air catalyst of primary Zn-air batteries, a high open-circuit voltage of 1.46V and excellent power density as well as operation durability were achieved.

Keywords: Atomic cobalt, Oxygen Reduction Reaction, Metal-air batteries

A02-P63

Defect Engineering of Molybdenum Disulfide to Tunable Hydrogen Evolution Behavior through Ion Irradiation

Engang Fu*[1,2], Peipei Wang[1,2], Cheng Sun[3], Hao Wang[3], Guifu Zou[3]
1. School of Physics, Peking University, Beijing 100871, China
2. State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China
3. Soochow Institute for Energy and Materials InnovationS & Key Laboratory of Advanced Carbon Materials and Wearable Energy Technologies of Jiangsu Province, Soochow University, Suzhou 215006, China.

Hydrogen evolution from water splitting is an efficient strategy related to clean energy and sustainable environment. Therefore, exploiting hydrogen evolution reaction (HER) catalysts has been actively encouraged. The layered MoS_2 is proposed to be the alternative HER catalyst due to its electrocatalytic H_2 properties as well as the low cost. To improve the electrocatalytic activity of MoS_2, designing and modifying the microstructure of catalyst is proposed for achieving extra-high activity and enhanced durability. Herein, we report an effective strategy for modifying the microstructure of MoS_2 by ion irradiation. Irradiation is extensively used in the field of semiconductors which can cause the microstructure and properties change via transferring high energies to the target

compounds. The induced damages and changes of microstructure in MoS_2 are controlled and can effectively improve the electrocatalytic activity.

The ultrathin MoS_2 nanosheets were prepared through a lithium intercalation and exfoliation method. Transmission electron microscope (TEM), X-ray diffraction patterns (XRD) and X-ray photoelectron spectroscopy (XPS), Raman spectra and electron Spin Resonance (ESR) spectra were used to characterize the microstructure of MoS_2 before and after irradiation. The ion irradiations were performed at room temperature using 3 MeV C ions by NEC 1.7 MV Tandem accelerator. A total fluence of 5 x $10^{12}\mathrm{cm}^{-2}$, 2 x $10^{13}\mathrm{cm}^{-2}$ and $5\mathrm{x}10^{13}\mathrm{cm}^{-2}$ was achieved at a constant beam current, respectively. The HER tests for different MoS_2 samples were carried out on a CHI 660E electrochemical workstation via a three-electrode electrochemical configuration in an N_2-purged 0.5 M H_2SO_4 electrolyte.

The tunable S-vacancy is well introduced to the basal plane of MoS_2 by ion irradiation. It is found that the ion fluence plays a major role in improving the HER performance of MoS_2. The different ion fluences can tune the number of the S-vacancy and amorphous phase on the basal plane of MoS_2. The ion-irradiated MoS_2 upon the fluence of 2 x $10^{13}\mathrm{cm}^{-2}$ exhibits the best HER performance with an onset potential of 76 mV and Tafel slope of 66 mV dec^{-1}. The experiments demonstrate more active sites caused by S vacancies from the basal plane mainly contribute to higher HER catalytic efficiency while more amorphous state restricts the performance of MoS_2. This effective and feasible approach of ion irradiation provides a platform to introduce the desirable vacancy for the other similar materials.

Keywords: Molybdenum disulfide, Ion irradiation, Electrocatalyst, Hydrogen evolution reaction, Sulphur vacancy

A02-P64

Hybrid Electrodes with High Capacity for Lithium Ion Battery Anodes

Siguang Guo*[1], Biao Gao[1], Kaifu Huo[1,2]
1.Wuhan University of Science and Technology
2. Huazhong University of Science and Technology

Lithium-ion batteries (LIBs) have attracted increasing attention in energy storage due to their superior energy density, operating voltage and cycle life [1-4]. In order to satisfy the increasing demand for high energy density application, candidates with high theoretical specific capacity have proposed to replace commercial graphite as anodes due to its low theoretical specific capacity of only 372 mA h g^{-1}. Herein, we introduce our recent work on the design and Li- ion storage properties of special nanostructures for high-performance LIBs anodes such as Si/C nanocomposites, conjointed Sn/C hollow spherical nanocomposite and pea-pod like Ge/C nanowires et. al [5-9]. Above nanostructured anodes with plentiful active sites for Li-ion storage as well as the structural integrity exhibit high specific capacity and good cycling stability, enabling their promising applications in next generation LIBs.

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Keywords: Lithium-ion batteries, Negative materials, Hybrid, Ⅳ group elements

A02-P65

Enhancing efficiency and stability of perovskite solar cells via a high mobility p-type PbS buffer layer

Qi Zhang*, Xiaolu Zheng, Guojia Fang
Wuhan University

Although the perovskite solar cells (PSCs) based on organic hole transport materials (HTMs) have demonstrated excellent photovoltaic performance, there are still some obstacles that limiting their future commercialization, one of which is the device

stability. Herein, we first report that depositing a (200) orientated PbS thin film upon organic HTMs as buffer layer can significantly enhance the stability and improve the performance of PSCs. The superior hole extraction efficiency of spiro-OMeTAD/PbS bilayer can balance the charge transfer and the hydrophobic nature of PbS could avoid the permeation of moisture. As a result, the PSCs with PbS buffer layer exhibited a better photovoltaic performance (a champion power conversion efficiency of 19.58%) with respect to the reference cells (18.79%), and maintained almost 100% of its initial PCE after 1000 h stored in ambient air. Furthermore, when suffer from some more severe conditions, the device with PbS retained 56% of its initial PCE after 96 h annealing at 85 °C, while only 25% for the reference cells. Our results provide a simple method to avoid the weakness of organic HTMs, and suggest that PbS thin film could be an alternative buffer layer material in PSCs to simultaneously improve the device stability and photovoltaic performance.
Keywords: Perovskite solar cells, PbS film, High mobility Buffer layer ,Stability

A02-P66

Defects and Interfaces on PtPb Nanoplates Boost Fuel Cell Electrocatalysis

Engang Fu*[1,2], Yanxia Liang[1,2], Yingjun Sun[3,4], Xinyu Wang[5,6], Xiaodong Wen[6], Shaojun Guo[4]
1. School of Physics, Peking University, Beijing 100871, China
2. State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China
3. College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, China.
4. Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, China.
5. College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.
6. State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan 030032, China.

Nanostructured Pt is the most efficient single-metal catalyst for fuel cell technology. Great efforts have been devoted to optimizing the Pt-based alloy nanocrystals with desired structure, composition and shape for boosting the electrocatalytic activity. However, these well-known controls still show the limited ability in maximizing the Pt utilization efficiency for achieving more efficient fuel cell catalysis. Herein, we report a new strategy for maximizing the fuel cell catalysis by controlling/tuning the defects and interfaces of PtPb nanoplates using ion irradiation technique. The defects and interfaces on PtPb nanoplates, controlled by the fluence of incident C^+ ions, make them exhibit the volcano-like electrocatalytic activity for methanol oxidation reaction (MOR), ethanol oxidation reaction (EOR) and oxygen reduction reaction (ORR) as a function of ion irradiation fluence. The optimized PtPb nanoplates with the mixed structure of dislocations, subgrain boundaries and small amorphous domains are the most active for MOR, EOR and ORR. They can also maintain high catalytic stability in acid solution. Our work highlights the impact and significance of inducing/controlling the defects and interfaces on Pt-based nanocrystals toward maximizing the catalytic performance by advanced ion irradiation strategy.

Besides, a novel structure is designed for the first time in PtPb NP by using 1MeV Kr^{3+} ion irradiation, and the PtPb NP with this structure has an excellent catalytic activity for MOR. In new structure, crystalline phase and amorphous phase co-existing on the surface simultaneously have been achieved for the first time and the crystalline phase is surrounded by the amorphous phase annularly to form crystalline/amorphous interface. The new findings show that the crystalline/amorphous interface in the novel structure plays an important role in improving catalytic activity, explained reasonably on the basis of the experimental measurements and theoretical calculation. Crystalline/amorphous interface can provide plenty of active sites by tuning the electronic structure of Pt atom and d-band center value, as a result, the atoms in crystalline/amorphous interface can activate the C-H bond and O-H bond enhancing the catalytic property. Meanwhile, the adsorption energy of hydroxyl and intermediates is optimized by the interface to facilitate the complete oxidization of small molecules.
Keywords: PtPb nanoplates; ion irradiation; interface; fuel cells

A02-P67

Fe Isolated Single Atoms on S, N Codoped Carbon by Copolymer Pyrolysis Strategy for Highly Efficient Oxygen Reduction Reaction

Zhi Li*
Tsinghua University

Iron/heteroatoms-doped carbon materials have emerged as one of the most promising candidates to replace noble metal based catalysts for highly efficient oxygen reduction reaction (ORR). Modulating the Fe-N_x active center to optimizetheir performance and understanding the catalysis at molecular level are highly desirable but remains a great challenge. Herein, a novel pyrrole–thiophene

copolymer pyrolysis strategy to synthesize Fe‐isolated single atoms on sulfur and nitrogen‐codoped carbon (Fe‐ISA/SNC) with controllable S, N doping is rationally designed. The catalytic efficiency of Fe‐ISA/SNC shows a volcano‐type curve with the increase of sulfur doping. The optimized Fe‐ISA/SNC exhibits a half‐wave potential of 0.896 V (vs reversible hydrogen electrode (RHE)), which is more positive than those of Fe‐isolated single atoms on nitrogen codoped carbon (Fe‐ISA/NC, 0.839 V), commercial Pt/C (0.841 V), and most reported nonprecious metal catalysts. Fe‐ISA/SNC is methanol tolerable and shows negligible activity decay in alkaline condition during 15 000 voltage cycles. X‐ray absorption fine structure analysis and density functional theory calculations reveal that the incorporated sulfur engineers the charges on N atoms surrounding the Fe reactive center. The enriched charge facilitates the rate‐limiting reductive release of OH* and therefore improved the overall ORR efficiency.
Keywords: Fe single atoms, S and N codoped carbon, oxygen reduction reaction, electrocatalyst

A02-P68

Resolving the Local Electrochemistry of Lithium-ion Battery Electrode Materials via ESM

Aolin Li*[1], Kai Pan[1], Yunya Liu[1], Chihou Lei[2], Jiangyu Li[3]
1. School of Materials Science and Engineering, Xiangtan University
2. Department of Aerospace and Mechanical Engineering, Saint Louis University
3. Department of Mechanical Engineering, University of Washington

Electrochemical strain microscopy (ESM) is a powerful tool to characterize the electrochemical activities with lithium ions in lithium-ion battery electrode materials. Recently years, ESM has been employed to understand the interaction between mechanics and electrochemistry in lithium battery. In order to analyze the mechanics and electrochemistry underneath a charged scanning probe, herein, we develop a numerical model based on experimental ESM mapping, spectroscopy, and relaxation. Our calculation results of ceria show well agreement with its ESM experimental observations, and the ESM response correlates with local concentration, diffusivity and elasticity modulus. The combination of ESM calculation and experiments paving ways for deep understand the electrochemistry in lithium-ion battery at nanoscale.
Keywords: Electrochemical strain microscopy; Lithium-ion battery; Electrochemical

A02-P69

Scalable synthesis of $Co_{0.5}Ni_{0.5}MoO_4$ double-shelled hollow spheres for high-performance supercapacitors and lithium-ion batteries

Wei Chen*, Lun Li
State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology

Binary metal molybdates have attracted sufficient research interest in supercapacitors (SCs) and lithium ion batteries (LIBs). Here we successfully synthesized the $Co_{0.5}Ni_{0.5}MoO_4$ double-shelled hollow spheres (DSHSs) using a simple and scalable spray drying method for the first. The as-synthesized $Co_{0.5}Ni_{0.5}MoO_4$ DSHSs exhibit a high capacitance of 731 F g^{-1} at 0.5 A g^{-1} and a superior capacitance retention of 80% at 5 A g^{-1} after 2000 cycles, as well as an excellent rate capability of 78% at 10 A g^{-1} in supercapacitors. Moreover, it also shows high discharge capacity of 1847 mAh g^{-1} (200 mA g^{-1}) at the first cycle, maintaining a high discharge capacity of 756 mAh g^{-1} after 1000 cycles and a good rate capability of 403 mAh g^{-1} at 5 A g^{-1} for LIBs. The enhanced electrochemical performance both in SCs and LIBs is ascribed to the synergistic contribution of the nickel and cobalt. Our work provides an effective strategy for the fabrication of various binary transition metal oxides or metal oxides for high-performance SCs and LIBs.
Keywords: $Co_{0.5}Ni_{0.5}MoO_4$ DSHSs, spray drying, supercapacitors and lithium ion batteries

A02-P70

Effect of different Rare Earth element (Gd+Y) on the microstructure and high temperature tensile properties of Mg-xGd-yY-0.5Zr alloys

HamidReza JafariNodooshan*, Xiaoqin Zeng, Dejiang Li, Wencai Liu, Guohua Wu, Wenjiang Ding
National Engineering Research Center of Light Alloy Net Forming and Key State Laboratory of Metal Matrix Composite, Shanghai Jiao Tong University, Shanghai 200240, China

In this study, the compositional dependence of the age hardening response and room and high temperature tensile properties of the Mg–*x*Gd–yY–0.5Zr alloys investigated. The results showed that the Mg-10Gd-5Y-0.5Zr alloy shows the optimum strength at room and high temperature among Mg-xGd-yY-0.5Zr alloys, the alloy shows the lower UTS than Mg-10Gd-3Y-0.5Zr alloy at room temperature but its high temperature mechanical properties is higher than that of Mg-10G-3Y-0.5Zr alloy. Mg-10Gd-5Y-0.5Zr alloy shows the UTS and YS value of 331 and 241 MPa at room temperature, however, the UTS and YS increased to 350 and 261 MPa with increasing the test temperature from room temperature to 150 °C, respectively. The alloy shows the UTS value of 225 MPa at 300 °C which is 50 MPa higher than that of Mg-10Gd-3Y-0.5Zr at the same temperature. The elongation of the alloy increased monotonically with increasing the test temperature and all alloy showed their maximum elongation at 300 °C. The superior high temperature tensile strength of the Mg–10Gd–5Y–0.5Zr alloy was mainly associated with solution strengthening and precipitation strengthening of β′ phases in Mg matrix. Especially β′ phase can hinder the dislocations movement at high temperature.

Keywords: Mg–Gd–Y–Zr alloy; High temperature; Precipitation hardening; Tensile properties

A02-P71

High specific capacity carbon coated silicon/graphene nanocomposite anode materials for Li-ion batteries

Si Xiao*, Xi Ke, Jun Liu, Zhicong Shi

New Energy Materials and Devices Department, School of Materials and Energy, Guangdong University of Technology

Silicon (Si) has been investigated as a promising high specific capacity anode material for lithium ion batteries (LIBs) to replace the commercially graphite. Unfortunately, the practical use of pure Si in LIBs is still hindered by the fast capacity fading due mainly to the large volume change and structural cracking upon repeated Li^+ insertion/extraction. Another problem is that structural cracking of electrode exposes the new surface of Si to deposit solid electrolyte interphase (SEI), which resulted in large irreversible capacity. In addition, the low intrinsic electronic conductivity of Si usually leads to large potential polarization and inferior rate-capability and thus lower reversible capacity.

In view of small volume change and excellent cyclablity of graphene and large lithium insertion capacity of Si, they were adopted as matrix and main active material respectively. New types of carbon coated silicon/graphene composites were prepared by methods of high energy ball milling and carbonization of organic materials.

The material prepared by high-energy ball milling at a speed of 500 rpm is small and relatively uniform, and the high-energy balling mill can generate high energy through collision. Si nanocrystals are uniformly dispersed in carbon and have a good stability. The capacity of the resulting composite materials can be achieved by controlling the ratio of Si and graphene, and the time of ball milling. XRD analysis shows that high-energy ball milling can produce nanocrystalline and partially amorphous Si， and generate electrochemically inert carbonized silicon (SiC). Electrochemical test results show that the material has a very high specific capacity (2200mA/g), which is due to the fact that the carbon carrier in the composite material can buffer the volume change in the process of Si intercalation with lithium, and at the same time provide good electrical contact for Si.

The sucrose-asphalt carbon coated silicon/graphene composites were prepared by carbonization of organics after high-energy ball milling. The volume change of Si in the cyclic process is absorbed by the sucrose-asphalt carbon, and the specific surface area of the ball mill material is greatly reduced, thereby reducing the irreversible capacity of the first cycle, and the columbic efficiency is as high as 84.25%.

Keywords: Li-ion batteries, silicon/graphene nanocomposite anode materials, high energy ball milling

A02-P72

Broadband antireflection sub-microstructures on 4H-SiC

Jun Yuan*, Xing Huang, Weijiang Ni

Beijing Century Goldray Semiconductor Co.Ltd

By using insufficient baked resist as etching mask, CENGOL team has developed a global initiative and cost-effective process for fabricating antireflective sub-macrostructures on SiC wafer’s surface. The etched sub-micro structure is a mesh-trenched pattern thus as the so called “mesh patterning etching”. The mesh patterning process is more time-effective than the nano-imprint lithography or e-beam lithography process. The impact of the RIE process conditions and post bake temperature of the resist film to the profile of sub-microstructures and the according surface reflectance has been investigated. Under optimized process conditions, a perfect mesh patterning sub-micro structures is formed upon a 4-inch 4H-SiC wafer surface. In the broadband range of 390-800 nm, the average

reflectance of the silicon carbide is dramatically suppressed from 40 % to around 8%.

Keywords: Silicon Carbide; sub-microstructure; surface antireflection; Intermediate Band Solar Cells;

A02-P73

Controllable Synthesis of Ultrathin CsPbBr3 Nanoplatelets and Their Reversible Transformation into Cs4PbBr6 Nanocrystals

Wei Zhai, Jing Lin*, Yang Huang*, Chengchun Tang
School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, P. R. China
Hebei Key Laboratory of Boron Nitride Micro and Nano Materials, Hebei University of Technology, Tianjin 300130, P. R. China
linjing@hebut.edu.cn; huangyang@hebut.edu.cn

Lead halide perovskite nanocrystals (NCs) have recently gained huge interest due to their outstanding optical and electronic properties, and thus have shown great potential for applications in light-emitting diodes (LEDs),1-5 photovoltaic cells,6, 7 photodetectors,8-10 etc. Due to the intrinsic instability and soft nature, lead halide perovskite NCs can be synthesized in a variety of sizes, shapes, and compositions,11-13 such as organic-inorganic hybrid perovskites CH3NH3PbX3 (X=Cl, Br, I)15-17 and all-inorganic perovskites CsPbX3 (X=Cl, Br, I)18, 19 in various morphologies (quantum dots,18 nanowires,12, 21 nanoplatelets,22, 23 nanocubes,24, 25 etc.). The versatility of perovskite crystal structure has become the great advantage of lead halide perovskite NCs for their functional applications.

Precise control over the morphology, structure and composition of lead halide perovskite NCs not only offers great opportunity for accessing novel nanostructures, but also allows for understanding the growth evolution of NCs and establishing their structure-property link. Since the pioneering work reported by Kovalenko group,18, 26, 27 the research on controllable synthesis of all-inorganic CsPbX3 NCs with tailored morphology and structure has attracted increased attention. In 2015, Kovalenko group reported the synthesis of CsPbX3 NCs by an air-free hot injection method. The halide compositions can be easily changed via ion-exchange transformations, resulting in the tunable photoluminescnece (PL) emission.18 Deng group developed a ligand-mediate reprecipitation method for manipulating the shape of CsPbX3 NCs. Diverse CsPbX3 NCs, including quantum dots, nanocubes, nanorods and nanoplatelets (NPLs), have been synthesized and show distinct shape-dependent PL emissions.20 Moreover, the Manna group reported interesting monolayer-level thickness control over CsPbBr3 NPLs to achieve thickness-dependent PL emission.28 Very recently, the chemical transformation of CsPbBr3 NCs to get a new kind of lead−halide depleted perovskite derivative, i.e. Cs4PbX6 NCs, has also attract much attention.29-31 The Cs4PbX6 phase has been considered as a type of zero-dimensional perovskite, showing a different insulator bandgap.32, 33

Although great efforts have been devoted to the controllable synthesis of lead halide perovskite NCs, many challenges still remain. The air-free hot injection method has been considered as the most mature approach for synthesis of CsPbX3 NCs.11, 18, 27, 34 However, the rapid reaction in very short time is not facilitated for the controllable synthesis. With the aim of precise control over such tiny NCs, a relatively mild crystal growth environment is favorable. 35 In this paper, we develop a facile solvothermal method for the controllable synthesis of CsPbBr3 NPLs and their transformation to Cs4PbBr6 NCs. The readily effective method results in the production of uniform CsPbBr3 NPLs in a large-scale. Owing to the sealed environment of the solvothermal method, there are no extra procedures for an inert atmosphere which are usually necessary in the other methods. 18, 20 In the solvothermal synthesis, the reaction between Cs-oleate and PbBr2 precursors can take place at relatively low temperatures and the kinetics of the reaction can also be depressed. As a result, we can succeed in achieving monodisperse CsPbBr3 NPLs with precisely tuned lateral sizes by simply adjusting the reaction times or temperatures. In addition, we demonstrate that the developed solvothermal method can be extended for further structure and composition control over the cesium lead halide NCs. A successful reversible transformation between CsPbBr3 NPLs and Cs4PbBr6 NCs can be achieved by simply changing the amount of Cs-oleate or PbBr2 precursors.

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A02-P74

High-performance lithium-sulfur batteries with a carbonized chitosan modified separator

Lei Tan, Xinhai Li*, Zhixing Wang, Huajun Guo, Jiexi Wang, Guochun Yan

School of Metallurgy and Environment, Central South University, Changsha 410083, China
Email: xinhaili_csu@126.com (X. Li); Fax: +86-731-88836633; Tel: +86-731-88836633

The development of lithium-sulfur (Li-S) batteries is limited by the polysulfide dissolution, leading to the serious crossover of polysulfide to Li anode, thereby reducing the cycle stability and cycle life of the batteries. To address this issue, here a carbonized chitosan (CCTS) modified separator is designed to restrain the shuttle effect of Li-S batteries. It shows that the CCTS is able to enhance the interfacial interaction between coating and polysulfide and provide a large surface area for absorbing polysulfide, and thus improving the electrical conductivity. It has been demonstrated that the Li-S cell constructed with the CCTS composite separator results in a reversible capacity of as high as 1058 mAh g-1 at 0.2 C and a low fading rate of 0.14% for 100 cycles. And during the rate test, Li-S cells can deliver a discharge capacity of 580 mAh g−1 at 2 C. The outstanding performance is attributed to a reduction in the crossover rate of polysulfide through the composite separator as a result of the polysulfide absorption by CCTS layer.

A02-P75

Mesoporous lamellar-shaped lithium-rich cathode material for lithium-ion batteries with exceptional rate capability and stability

Min Li [1, 2], Yi Zhou[1, 2], Xiaoyan Wu[2], Lei Duan[2], Chunming Zhang [2], Fang Zhang[2], Dannong He[1, 2*]
1. School of Material Science and Engineering, Shanghai Jiao Tong University, No.800 Dongchuan Road, Shanghai, 200240, PR China
2. National Engineering Research Center for Nanotechnology, No.28 East Jiangchuan Road, Shanghai, 200241, PR China

With the development of society, the problem of energy has become more and more serious. Lithium-ion battery, acting as the new energy, has a lot of advantage, such as environment-friendly and portability. Although the lithium-ion battery has been researched for many years, the low energy density and severe cycle performance are also hardly meet the current requirement. Lithium-rich oxide layer material, which could exhibit the over 250 mAh g-1 when the charge voltage reaches the 4.8 V, has become more and more attractive to researcher. However, the drawbacks of encountering structural reconstruction, sharp voltage decay during cycling as well as low packing density still exist, which retard their further commercial development. This paper presents a novel approach to construct mesoporous lamellar-shaped Li1.2Mn0.54Ni0.13Co0.13O2 particles. One crucial step during the synthetic process is the usage of Hexadecyl trimethyl ammonium Bromide (CTAB) and Hexamethylenetetramine, which act as the precipitant and nucleate. And the key control parameter is time and temperature of hydrothermal reaction, which directly affects the morphology and size of particles. Of particular note is the desirable architecture which not only inherits the merits of hollow structures but also facilitates the tight particles packing. Owing to these advantages, mesoporous lamellar-shaped Li1.2Mn0.54Ni0.13Co0.13O2 exhibits the excellent discharge capacity and cyclic stability. Under the 0.5 C rate, its initial discharge capacity reaches the 236.13 mAh g-1, and the capacity retention above 85.3 % over 150 cycles. These results reveal that structural design of cathode materials play a pivotal role in increasing the electrochemical performance of lithium-rich oxide layer material.

A02-P76

Controllable Synthesis of Non-Stoichiometric Copper Chalcogenide Nanocrystals with Tunable Near-Infrared Localized Surface Plasmon Resonance Absorption

Dongxu Zhu*[1], Feng Teng[2], Aiwei Tang[1,2]
1. Department of Chemistry, School of Science, Beijing JiaoTong University
2. Key Laboratory of Luminescence and Optical Information, Ministry of Education, Beijing JiaoTong University

Localized surface plasmon resonances (LSPRs) are typically observed in noble metal nanostructures due to the presence of free electrons. Very recently, some semiconductor nanocrystals including copper-deficient copper chalcogenides and oxygen-deficient metal oxides also show LSPR behaviors in the near-infrared region due to the existence of free carriers arising from non-stoichiometries. In this work, we will introduce some progress of our group in the controllable synthesis of non-stoichiometric copper chalcogenide and their tunable LSPR absorption. A colloidal chemical method was developed to synthesize binary $Cu_{2-x}S$, $Cu_{2-x}Se$ and ternary alloyed $Cu_{2-x}S_ySe_{1-y}$ nanocrystals, whose morphology, size and crystal structure could be tuned by varying the reaction conditions, such as reaction time, temperature and surface ligands.

Particularly for $Cu_{2-x}S$, we could obtain CuS, Cu_7S_4 and $Cu_{31}S_{16}$ nanocrystals with different phases just by varying the Cu/S feeding ratios, in which the sulfur powder was used as S precursors. However, the CuS nanocrystals were post-treated by

1-dodecanethol, the crystal structure could transit from CuS to $Cu_{31}S_{16}$. Accordingly, the LSPR absorption exhibited a strong dependent on the crystal structure and surface ligands, which could be tuned from 1140 to 1910 nm. Furthermore, ternary alloyed $Cu_{2-x}S_ySe_{1-y}$ nanocrystals were synthesized by using sulfur powder and 1-dodecanethiol as sulfur sources, which could be transformed from Se-rich cubic berzelianite to S-rich monoclinic djurleite phase with an increase of sulfur content. Correspondingly, the as-obtained alloyed ternary nanocrystals synthesized using 1-dodecanethiol could be tunable over a broad range of 1250 nm, but the region of the red-shift for the products synthesized using sulfur powder could reach up to 200 nm, which indicated that the different sulfur sources played an important role in the difference of the LSPR tuning. These findings provide more opportunities for tuning the near-infrared (NIR) LSPR absorption of copper chalcogenide nanocrystals in a wide range.

Keywords: LSPR; NIR; $Cu_{2-x}S$ NCs; $Cu_{2-x}Se$ NCs; Alloyed $Cu_{2-x}S_ySe_{1-y}$ NCs

A02-P77

石墨烯负载纳米银复合材料的制备及性能研究

周懿涵
济南大学

纳米银线因其具有的良好的导电性、大的比表面积、量子效应和小尺寸效应，引起人们的广泛的研究和应用。银线利用石墨烯的优势与石墨烯复合具有更优异的电子和催化性能。本文应用 Hummer 法制备氧化石墨烯，采用多元醇法通过控制反应时间、反应温度、AgNO3 和 PVP 的比例、等因素制备不同形貌的纳米银线。实验结果表明：制备的氧化石墨烯在扫描电子显微镜下呈现单层状态，表面出现不规则褶皱；随反应时间的增加，出现不同形貌的银产物，生成的纳米银线的直径也变得不均匀；随反应温度的升高，产物中的银颗粒明显减少，银线直径更趋向于均匀化，但是直径会增大；综合各影响因素，制得直径均匀、颗粒含量少、直径在 20nm 左右的高长径比纳米银线的反应条件是：反应温度为 150℃、反应时间 10h、AgNO3:PVP=1:3、NaCl 浓度为 300μmol/L、反应溶液呈中性。测量不同形貌的石墨烯/纳米银对大肠杆菌和金黄色葡萄球菌的抑菌直径可以发现：不同形貌的纳米银与石墨烯复合的抑菌效果好，银立方体优于银颗粒和纳米银线。

关键词：石墨烯；纳米银线；微观形貌；抑菌性能

A02-P78

In situ Growth of Heterostructured Sn/SnO Nanospheres Embedded in Crumpled Graphene as an Anode Material for Lithium-ion Batteries

Jing-Feng Wang[1], Dan-Nong He [1,2]
1. National Engineering Research Center for Nanotechnology
2. School of Materials Science and Engineering, Shanghai Jiao Tong University

Towards the direct formation of heterostructured tin-graphene composites, one-step preparation and simultaneous combination of graphene and Sn nanoparticles are of particular difficult. In our current work, we report the situ growth of Sn/SnO core-shell heterostructured nanospheres within the crumpled graphene based on a new strategy of the calcinations of tin oleate coating on the crystal surface of sodium carbonate for the first time. It is worth noting that Sn/SnO nanospheres and crumple graphene are acquired simultaneously without external forces involved, making the in-situ growth process simple and environmentally friendly. The obtained composite exhibits large specific capacity, excellent cycling stability and high rate capability as an anode for LIBs, ascribed to the synergistic effects combining the formation of Sn/SnO heterostructure and the growth of graphene layers. This work provides a simple but efficient route for the controlled fabrication of metal/metal oxides/graphene heterostructures with promising applications in the fields of lithium-ion batteries or electronics.

Keywords: Sn/SnO nanospheres, crumpled graphene, in-situ growth, one-step synthesis, lithium ion batteries

A02-P79

Facile In-Situ Synthesis of Crystalline VOOH-Coated VS_2 Microflowers with Superior Sodium Storage Performance

Wenbin Li, Jianfeng Huang, Liangliang Feng, Liyun Cao
School of Materials Science & Engineering, Shaanxi University of Science and Technology

仅发表论文

A02-PO-01

Electric field driven Resistive Switching Behavior in the La0.7Sr0.3MnO3/BaTiO3 multiferroic heterostructure

Tingxian Li [1], Ruolan Li [2]
1. Anyang Normal University
2. Tangyin county No 1 middle school

Recently, memristors and memristive devices have aroused considerable research interests because of their favorable scalability, multilevel storage capability, synapse-like behavior, dynamic responses, and low power consumption. Today many efforts have been employed to the development and study of the new memristive materials, which was proposed on the basis of electric field induced resistance (EPIR) change effect discovered in numerous transition-metal-oxides, such as perovskite manganites, titanates, zirconates and niobic oxides. In the EPIR materials, resistance of the oxides can reversibly switch between two stable resistive states with applied short electric pulses of different polarities, and the modified resistance retains even after removing the pulse source.

As we knew, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is a kind of manganite exhibiting a metallic conduction near the ambient temperature, LSMO exhibits a significant magnetoresistance effect near the room temperature because of its high Curie temperature 350 K. This suggests a possibility to group the EPIR chang and magnetoresistance properties into the same system. Furthermore, LSMO is the generally used ferromagnetic layer for the ferromagnetic/ferroelectric (FM/FE) layered multiferroic heterostructure. These layered multiferroic heterostructures are especially promising for the future memory devices due to its lower leakage current and superior poling properties than that of another multiferroic structure, which is at the center of applications for the design of new multifunctional device architectures such as multiple-state memories, multiresponsive sensors and actuators, etc.

Based on these considerations, we performed a systematic study on the EPIR change in the LSMO/BTO multiferroic heterostructure. In this work, the resistive switching behavior of the $La_{0.7}Sr_{0.3}MnO_3/BaTiO_3$ (LSMO/BTO) multiferroic heterostructure is studied through controlling the electric field across ferroelectric BTO layer. The $La_{0.7}Sr_{0.3}MnO_3$ film was first epitaxially deposited on (001)- oriented $LaAlO_3$ (LAO) single-crystal substrate (10mm×5mm×0.5mm) by pulsed laser deposition technique. Then, the ferroelectric BTO film was grown onto the bottom LSMO layer. Here, LSMO and BTO are widely used for the colossal magneto resistive (CMR) and ferroelectric (FE) materials in the information technology, respectively.

Epitaxial growth of LSMO/BTO films have been confirmed in the analysis of X-ray diffraction θ–2θ scan. The LSMO and BTO films are of single phase and highly c-axis orientated, with a strong peak identified as LSMO and BTO (00*l*) besides the LAO (00*l*) diffraction peak. The full width at half maximum (FWHM) of the LSMO (002) peak is as narrow as 0.28 in the rocking curve, as given in the inset of Fig. 1, indicating an especially high degree of in-plane atomic ordering of the film.

The magnetic and the electric properties of the heterostructure had been investigated. Magnetic properties are mainly dominated by LSMO layer. The ferromagnetic hysteresis loop at 300 K shows the typical characteristics of soft ferromagnet. The saturated magnetization (Ms) is around 360 emu/cm^3. It reveals that the film deposited on LAO substrate possesses good room-temperature ferromagnetic property.

Good room-temperature ferroelectric property is verified. For the film grown on LAO substrate, the remnant polarization (P_r) of 13.1 $\mu C/cm^2$, and the electrical coercive field (E_C) of 43.2 kV/cm are obtained, respectively.

Furthermore, the variations of resistivity and metal-insulator transition temperature T_{MI} of LSMO layer, which is induced by the external electric field are studied. The temperature of metal-insulator phase transition (T_{MI}) for the LSMO film is 243K when there exists a positive electric field. The value of T_{MI} is lower (260K) and the resistivity is higher than that the other one. A field effect MIS structure composed of Ag electrodes, BTO and LSMO layers is formed when an electric field is applied to the BTO layer. It is well known that, the LSMO film is a kind of P-type semi conductive material whose main charge carrier is hole. When a negative direction electric field is applied to the BTO layer, which will result in the accumulation of the hole and increase the carrier concentration in the LSMO surface layer. Another kind of circumstance, when a positive direction electric field is applied to the BTO layer, which will result in the depletion of the hole and decrease the carrier concentration in the LSMO surface layer. Therefore, the resistivity of the LSMO film with negative applied voltage across BTO layer is lower than that of the other one.

Moreover, we all know the LSMO is a ferromagnetic material with 100% spin polarizability. The accumulation or depletion of the carriers on the LSMO surface lead to the increase or decrease spin-polarized carriers concentration, respectively. Finally, it increases the surface magnetism and the electron transition probability for the heterostructure with negative electric field across BTO layer, which decrease the corresponding resistivity of LSMO layer.

In conclusion, we have studied the effect of electrical field on the resistive variation of LSMO/BTO heterostructure. A distinctive feature is that the transport behavior of the LSMO film is sensitive to external field cross BTO, and a switching of the resistance between two definite resistive states can be induced by electric pulses of different polarity. It provides a way for the development of new kinds of electronic devices, such as nonvolatile random-access memories, sensors and memristive devices, etc.

Keywords: magnetoelectric effect, multiferroic, FM/FE bilayer heterostructure, pulsed laser deposition

A02-PO-02

Effect of Deposition pressure and Substrate Bias on Microstructure and Properties of Nickel Alloy Coatings Deposited by Magnetron Sputtering

Hao Huang*[1], Mao Wen[2], Minjuan Wang[1], Hu Li[1], Chuan Xie[1], Xu Huang[1]
1. Beijing Institute Of Aeronautical Materials
2. College of materials science and engineering, Jilin University

In the course of preparation of SiC continuous fiber reinforced nickel matrix composites (SiC_f/Ni) by fiber-coating method, it is one of important procedure to deposit nickel alloy coatings onto SiC fibers by magnetron sputtering. Sputtering pressure and substrate bias can control the energy of incoming atoms and ions, respectively. Thus the influences of sputtering pressure and substrate bias (V_b) on microstructure, morphology, stress and hardness for Nickel 738 alloy coatings are explored by X-ray diffraction, atomic force microscope, surface profiler and nanoindenter. The experimental results show that all coatings exhibit a strong cubic (200) preferred orientation, in which the gain size drops with increasing deposition pressure, while gain size first increases and then decreases with increasing V_b. Both low deposition pressure and high V_b are beneficial to smooth the surface by overcoming the shadow effect. Compressive stress is helpful to maintain the integrity of precursor wires. When only -30 V bias is applied to substrate, compressive stress cannot be obtained by varying deposition pressure, but by increasing V_b compressive stress is achieved above -160V, meanwhile, realize good adhesion between Nickel 738 coating and SiC fiber. Hardness is strongly dependent on the incoming atoms or ions, and increases with decreasing deposition pressure or increasing V_b.

Keywords: Nickel Alloy coating; Precursor wire; Magnetron Sputtering; Stress; Structure

A02-PO-03

Effect of carbonization temperature on the structure and electrochemical properties of PAN based carbon felt

Huan Zhang*[1,2,3], Yi Tan[2,3], Xudong Luo[1], Na Chen[1]
1. Liaoning University of Technology
2. Dalian University of Technology
3. Key Laboratory of Materials Modification by Laser, Ion and Electron Beams

Polyacrylonitrile (PAN)-based carbon felts synthesized in the temperature range of 1000-1800℃ are investigated in terms of their structure and electrochemical properties for iron-chromium redox flow battery (ICRFB). The structure properties of the samples were characterized by SEM, XRD, Raman, FT-IR and elemental analysis. The results reveal that increasing the carbonization temperature can enhance the graphitization degree. However, different results were shown on the electrocatalytical properties of the electrodes towards iron-chromium redox couples. Electrochemical behavior was evaluated by cyclic voltammetry and electrochemical impedance spectroscopy measurements in a three electrode electrolytic cell. The carbon felts carbonized at 1400℃ and 1600℃ exhibit the best electrochemical activities towards the Fe^{2+}/Fe^{3+} redox reaction, while are the carbon felts carbonized at 1200℃ and 1800℃ towards the Cr^{3+}/Cr^{2+} redox reaction. It is further demonstrated that the energy efficiency of the ICRFB with the electrodes carbonized at 1800℃ reaches 82.87% at 60 mA/cm^2, which is 7.85% higher than that of the ICRFB with the electrodes carbonized at 1000℃. The dominant factor of ICRFBs with carbon felt electrodes carbonized in the temperature range of 1000-1800℃ is identified to be graphitization degree rather than electrochemical activity.

Keywords: PAN-based carbon felt;carbonization; graphitization degree; electrochemical activity; iron-chromium

A02-PO-04

Effect of Temperature on Warping Characteristic of Polyetherimide in Fused Deposition Molding

Ding Liu*, Ye Chen
Material science and Engineering School, Donghua University

Polyetherimide (PEI) have been intensively used for many applications due to their attractive properties. The increasing demand of PEI is driving novel manufacturing processes to be in short manufacturing cycle time and low production cost, which is difficult to realize in general molding processes. Fused deposition modeling (FDM) is a powerful additive manufacturing process, and has attracted more attentions, due to its low cost, simple forming process, and ability to directly form 3D parts.PEI is a thermal plastic, and it can be used for FDM process. However, its high melt temperature and warping characteristic limited PEI FDM process. During deposition process, inner stresses increased by layer contraction, strongly affects the prototype size precision. Under the effect of inner stress, the created prototype deformed, displaying as a warpingedge and inner-layer delaminating or cracking. Temperature has a great influence on the warping behavior of the prototype. In this paper, the effect of temperature on PEI warping characteristic in FDM is studied, including nozzle temperature, baseplate temperature, and ambient temperature. The results showed that higher ambient and baseplate temperature is useful for reducing the warp rate of products, while excessive nozzle temperature will increase the warp rate of the prototype.

Keywords: polyetherimide, temperature, warping, fused deposition modeling

A02-PO-05

Preparation of porous CoS_2 nanostructures for highly efficient electrocatalytic hydrogen evolution

Shancheng Yan*, Ka Wang, Haizeng Song, Xin Xu
Nanjing University of Posts and Telecommunications

In response to global energy and environmental issues, development of efficient and robust earth-abundant electrocatalysts for hydrogen evolution reaction is particularly important. In this study, a facile hydrothermal method is developed to synthesize of porous CoS2 nanostructures by sulfur powder and thiourea as sulfur sources on carbon cloths for highly efficient hydrogen evolution reactions. The huge load of CoS2 on carbon cloth，their unique porous nanostructures made CoS2 nanomaterials have excellent electrocatalytic properties. The remarkable HER catalytic performance was achieved with -67 mV at a current density -10 mA cm-2 and the Tafel slope 62 mV dec-1 in 0.5 M H2SO4 solution. The overpotential of HER only lost 2mV after 1000 cycles with remarkable stability, which opens up a low cost and scalable route to fabricate transition metal-based materials for application in advanced fields.

A01-PO-06

Composite piezoelectret for flexible and self-powered pressure sensor

Bo Wang*, Gang Zhang, Qi Liu, Gang Lu
School of Electrical Engineering and Automation, Luoyang Institute of Science and Technology

Harvesting energy from ambient environment for powering decentralized sensors represents a fascinating tendency for the next-generation electronic devices. To meet the critical demands for continuously personalized health monitoring, an ultrasensitive pressure sensitivity and flexibility are highly desired. In this work, we report a composite piezoelectret for flexible and self-powered pressure sensor (FSPS) using hot-pressing method. By constructing micron-sized voids in the composite films of fibrous polytetrafluoroethylene (f-PTFE) and fluorinated ethylene propylene (FEP), and combination with superior negative charges affinity, exceptional flexibility and sensitivity can be achieved. The FSPS shows wonderful quasistatic piezoelectric efficient d33 (~ 6300 pC N-1) with negligible fluctuation more than 100 days, and therefore remarkable sensitivity (7380 pC N-1) with excellent linearity in the subtle-pressure regime (< 1 kPa) is desired. In addition to ultrahigh sensitivity, fast response time of 50 ms and very low limit of detection of 5 Pa, the FSPS also features homogeneity and high stability. Furthermore, the FSPS owns the capability for detecting human motions such as wrist stretching, chest respiration, cheek motion and eyes blinking. It can be also used for monitoring human radial artery pulse. By virtue of easy processibility in large scale, light weight, and low cost, the FSPS is especially suitable for mass production and flexible electronics, indicating their promising applications in artificial intelligence and mobile healthcare monitoring systems.

A01-PO-07

Aging behavior of an AlCrMoTiZr high-entropy alloy prepared by powder metallurgy

Bo Ren*, Rui-feng Zhao
Henan Institute of Engineering

A high-entropy alloy, AlCrMoTiZr, was synthesized using a well-developed powder metallurgy process. The alloy ingot was heat treated for 12 h at 700–1000 °C to investigate the effects of aging treatment on the microstructure and hardness of the high-entropy alloy. The as-cast alloy exhibited a mixture of the dendrite (Cr, Mo)-rich with a body-centered cubic (BCC) phase and the inter-dendrite (Al, Zr)-rich with a hexagonal close-packed phase. The aged alloy showed a peak hardness of 656 HV at 800 °C and then softened after annealing at 900 °C. Age hardening of the alloy was mainly attributed to precipitation strengthening at 800 °C. Formation of ZrO2 and decomposed BCC phase were the main reasons for the softening.

A01-PO-08

Structure and property of CrCuFeMnNi high-entropy alloy produced by mechanical alloying

Ruifeng Zhao*[1,2], Bo Ren[2], Zhongxia Liu[1]
1. Zhengzhou University
2. Henan Institue of Engineering

CrCuFeMnNi high entropy alloy (HEA) powder was fabricated using mechanical alloying. Effects of milling time and subsequent annealing on the structure evolution were investigated. After 50 h of milling, CrCuFeMnNi HEA powder consists of FCC phase and minor BCC phase. The crystallite size and strain lattice of 50 h-ball-milled CrCuFeMnNi HEA powders was 12 nm and 1.02%, respectively. The 50 h ball milled alloy powder exhibits refined morphology and excellent chemical homogeneity. The solid solution structure of CrCuFeMnNi HEA powder transforms to FCC1 and FCC2 phase and minor s phase when annealled at 700 oC and maintain the stable structure when the annealing temperature was up to 900 oC. The saturated magnetizations and remanence ratio of the 50 h-ball-milled CrCuFeMnNi HEA powder are respectively 16.1 emu/g and 15.4 % and exhibit a good soft-magnetic propertiy.

A01-PO-09

Enhanced Electrochemical Performance of Layered Lithium-rich Cathode Materials by Surface Fabricating with Spinel Structure

Zeliang Yang*[1], Liying Bao[1,2], Lai Chen*[1], Yuefeng Su*[1,2,3], Yun Lu[1], Weikang Li[1], Zhe Ji[1], Shi Chen[1,2,3], Feng Wu[1,2,3]
1. School of Materials Science & Engineering, Beijing Key Laboratory of Environmental Science and Engineering, Beijing Institute of Technology, Beijing, 100081, China
2. National Development Center of High Technology Green Materials, Beijing, 100081, China
3. Collaborative Innovation Center of Electric Vehicles in Beijing, Beijing 100081, China

The layered Li-rich cathode material is one of the most promising cathode materials due to its much higher specific capacity and energy density than the commercial counterparts. The spinel structure was fabricated on the surface of the lithium-rich material and explored its effect on the pristine material $Li_{1.2}Mn_{0.6}Ni_{0.2}O_2$. The modified material with 3 *wt*% coating contents exhibited the best electrochemical performance. Its initial discharge specific capacity was 253.9 mAh/g and the initial coulomb efficiency was 78.35% at a 0.1C (1C=250mAh/g), exceeding the corresponding 224.6 mAh/g and 74.6% of the pristine material. The specific capacity and 100th retention at 1C rate had increased from 138.4 mAh/g and 87.5% of the pristine material to 158.7 mAh/g and 90.9% of the modified sample. The enhanced electrochemical performance should be attributed to the spinel structure, who not only stabilized the electrode/electrolyte interface but also provided 3D Li^+ diffusion channels. This conclusion was confirmed by analysis of XRD (X-ray diffraction), TEM (Transmission electron microscope) and electrochemical tests.

A01-PO-10

Review on the Flexible Electrode Assembled from Different Microstructures

Yingna Jia*[1], Xingxing Liu[1], Shuangyi Zhao[1], Yun Lu[1], Yuefeng Su[1,2,3], Lai Chen[1], Shi Chen[1,2,3], Feng Wu[1,2,3]
1. School of Materials Science & Engineering, Beijing Key Laboratory of Environmental Science and Engineering, Beijing Institute of Technology, Beijing 100081, China
2. National Development Center of High Technology Green Materials, Beijing 100081, China
3. Collaborative Innovation Center of Electric Vehicles in Beijing, Beijing 100081, China

With the development of wearable flexible electronic equipment, flexible electrochemical energy storage devices that can provide high energy and high power have drawn more attention. As for core component of flexible energy storage devices, flexible electrode should not only have basic mechanical flexibility, but also possess excellent electrical conductivity and skeleton support capability. With the deep researches on the flexible electrode, materials such as carbon nanotubes, carbon nanofibers, carbon cloth, polymer, metal compounds were introduced and combined into different form with each other to show flexibility. This paper classified different assembly methods for fabricating flexible electrode with different microstructures, including the stacked structure, foam structure, weave structure, grafting structure, etc. This paper also carried on the summary of quantitative evaluation of the flexibility. Finally, the future development and the major challenges for the flexible electrode are prospected.

A01-PO-11

Stabilizing the Pseudo-Cubic RbPbBr3 Perovskite Nanocrystals through Cs+ Substitution

Jiawen Xiao*, Yuan Liang, Siyu Zhang, Yujing Li, Qi Chen
Beijing Institute of Technology

The ABX_3-type halide perovskite nanocrystals (NCs) have been a hot topic recently due to their fascinating optoelectronic properties. A consensus has been reached on that A-site ion plays an essential role in the photophysical and chemical properties, such as photoluminescence quantum yield and chemical stability. The pursuit of halide perovskite materials with diversified A-site species would deepen the understanding on the structure-property relationship of the perovskite family. Herein, we attempt to synthesis the Rb-based perovskite NCs. We discover that the partial substitution of Rb^+ by Cs^+ helps to stabilize the pseudo-cubic-phase $RbPbBr_3$ NCs at low temperature, which otherwise can only be obtained at high temperature. The inclusion of Cs^+ into $RbPbBr_3$ lattice results in highly photoluminescent $Rb_{1-x}Cs_xPbBr_3$ NCs. With the increasing doping amount of Cs^+, the bandgap of $Rb_{1-x}Cs_xPbBr_3$ NCs decreases, leading to the red shift of photoluminescence peak. The stability study shows that the $Rb_{1-x}Cs_xPbBr_3$ NCs (x=0.4) are highly stable in ambient condition. This work demonstrates the high structural flexibility and tunability of halide perovskite materials through A-site doping strategy and sheds light on the optimization of perovskite materials for high-performance optoelectronic devices.

A02-PO-12

Supercapacitor Charateristics of NiO Synthesized by Deposition Transformation

Xinglei Wang*, Xiuling Yan
Xinjiang Laboratory of Phase Transition and Microstructure in Condensed Matters, College of Chemical and Environmental Science, Yili Normal University, Yining 835000 China

As an electrode material for supercapacitors, NiO has become a research hotspot in the field of electrochemical energy storage because of its high energy density and good cycling performance. In this paper, the $Ni(OH)_2$ precursor was prepared from nickel nitrate with cetyltrimethyl ammonium bromide (CTAB) as dispersant. The powder of NiO was prepared by annealing, and the effects of reaction conditions on the morphology and electrochemical properties of NiO were studied. The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), cyclic voltammetry (CV), constant current charge-discharge and AC impedance (EIS) method. The results show that the prepared NiO has typical pseudo-capacitance characteristics. In a dispersing agent of 0.8 mol L^{-1} CTAB, the specific capacitance of the NiO single electrode, which was obtained by annealing at 300 ^oC, is up to 501 F g^{-1} at 3 mA.

A02-PO-13

The Effect of Fluorine-containing Additive on the Electrochemical Properties of Silicon Anode for Lithium Ion Batteries

Jing Wang*, Xiaohang Yang
Beijing Institute of Technology

Silicon anode is a promising candidate as an alternative to conventional graphitic anode in lithium-ion batteries. In this work, silicon anode was modified by NH4F using a facile method in air. The concentration of NH_4F on the electrochemical performance is systematically checked. The 5 wt% NH4F-modified silicon anode exhibits enhanced capacities and rate performances, the first discharge specific capacity is 3958 mAh/g with 86.45% as the coulomb efficiency at 100mA/g. The capacity can maintain at 703.3 mAh/g after 50 cycles, exhibiting a much better cycle stability than pristine silicon anode (329.9 mAh/g after 50 cycles). SEM

images confirm that the addition of NH4F can alleviate the volume expansion of silicon, and X-ray photoelectron spectroscopy demonstrates that LiF can be created at the surface that is beneficial to the stability of solid-electrolyte interphase (SEI) membrane.

A02-PO-14

Influence of Calcination Temperature on structure and electrochemical behavior of $LiNi_{0.83}Mn_{0.06}Co_{0.11}0O_2$ Cathodes for Lithium-Ion Batteries

Jing Wang*[1,2,3], Danhua Li[1], Ran Wang[1], Shi Chen[1,2,3], Yuefeng Su[1,2,3], Ang Gao[1], Feng Wu[1,2,3]
1. Beijing Key Laboratory of Environmental Science and Engineering, School of Materials Science and Engineering, Beijing Institute of Technology, Beijing 100081, China
2. Collaborative Innovation Centre for Electric Vehicles in Beijing, Beijing, 100081, China
3. National Development Centre of High Technology Green Materials, Beijing, 100081, China

Nickel-rich layered oxides (Ni ≥ 80%) are considered as a very promising cathode material for lithium-ion batteries because of its high energy density and low cost. However, its cycling performance is seriously influenced by the synthesis condition, especially the calcination temperature. Herein, the layered Ni-rich $LiNi_{0.83}Mn_{0.06}Co_{0.11}O_2$ (LNMCO) cathodes were prepared by calcining the mixture of $Ni_{0.83}Mn_{0.06}Co_{0.11}(OH)_2$ precursor (co-precipitation method) and Li salts ($LiOH{\cdot}H_2O$) at the range of 700-800℃ in an oxygen atmosphere. The morphology, surface chemistry and crystal structure of different LNMCOs were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), transmission electron microscopy methods (TEM) and X-ray photoelectron spectroscopy (XPS). The electrochemical performance were measured by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The results indicated that the cycling performance of LNMCOs was heavily depended on the calcining temperature. Therefore, exploring the optimal calcination temperature of Li $Ni_{0.83}Mn_{0.06}Co_{0.11}O_2$ has a critical effect on its commercial application.

A02-PO-15

Effect of Unsaturated Sn Atoms on Gas-Sensing Property in Hydrogenated SnO_2 Nanocrystals and Sensing Mechanism

Yukun Yuan*, Qin Du, Yan Ren, Junfang Liu, Bin Liu, Hua Zhao, Heqing Yang
Shaanxi Normal University

Sensing reaction mechanism is crucial for enhancing the sensing performance of semiconductor-based sensing materials.

Herein, we demonstrated the enhanced volatile-organic-compound sensors based on the hydrogenated SnO_2 nanocrystals for the first time. The hydrogenated SnO_2 nanocrystals displayed far higher response towards ethanol, methanol and triethylamine than SnO_2 samples without hydrogenation, and the gas-sensing sensitivity was further increased with the hydrogenation time.

The excellent gas-sensing performance arises from the increased density of the unsaturated Sn atoms with dangling bonds through hydrogenation, a concept of the unsaturated Sn atom serving as an active site for the sensing reaction is thus proposed, and a new sensing reaction mechanism is described in detail at atomic and molecule level for the first time.

Sensing properties of other metal oxide sensors and catalytic activity of other catalysts may be improved by using the hydrogenation strategy. The concept of the surface unsaturated metal atoms serving as active sites may be very useful for understanding the sensing and catalytic reaction mechanisms and designing advanced sensing sensors, catalysts and photoelectronic devices.

A02-PO-16

De novo designed acoustic & magnetic co-drive contrast for both molecular imaging and drug delivery

Tingting Zheng*[2,1], Yun Chen[1,2]
1. Peking University
2. Shenzhen PKU-HKUST Medical Center

Silica coated magnetite (Fe_3O_4@SiO_2) core-shell nanoparticles (NPs) has great potential in preclinical studies to be applied as magnetic resonance imaging (MRI) contrast agents. However, according to strong magnetism property of Fe_3O_4 core, higher concentration of Fe_3O_4@SiO_2 always ends up with serious aggregations. Poor aqueous stabilities of these nanoparticles limit their applications. Here, a pleiotropic micro nano-carrier is reported for both drug delivery and magnetic resonance imaging. In brief, Fe_3O_4@SiO_2 nanoparticles with high colloidal stability have been synthesized. Average size of MNPs are around 220 nm, with 20 nm Fe_3O_4 NPs as seeds in core. We achieve the system's colloidal stabilities by encapsulating these magnetic NPs (MNPs) into

Ginsenoside Rg_3-microbubbles, yielding M-RMbs. Here Rg_3 is a therapeutic compound that has been observed in cell models as having an inhibitory effect on the cell growth of various cancer cells. In addition to its therapeutic effect, it is adopted in our system also as tumor targeting motif in model of colon cancer, and as water soluble block improving surface stability for MNPs. All these core-shell MNPs are characterized by X-ray diffraction (XRD) and UV-Vis adsorption spectra. Finally, targeted molecular imaging of these M-RMbs is tested via bioluminescence imaging, ultrasound imaging and MRI imaging systems. All results points out that the monodispersed M-RMbs are promising micro- nano-carriers which can be applied as both a pleiotropic contrast and a drug carrier for colon cancer.

A01-PO-17

Inorganic electron-transporting materials in perovskite-based solar cells

Weidan Li*, Qing Luo, Xiong Yin, Leyu Wang
Beijing University of Chemical Technology

Compared with conventional photovoltaic devices, perovskite solar cells have attracted great attention due to their high efficiency and solution processing [1]. Each layer can affect the power conversion efficiency (PCE) of the device. A compact electron-transport layer (ETL) is generally used in device to transport electrons and block holes. Our previous studies revealed: (1) The compact TiO2 layer doped with Nb5+ or Ru3+ can result in a high PCE of device. The enhanced performance was attributed to the decreased selective contact resistance and increased charge recombination resistance [2]; (2) When a zinc-rich ternary oxide TiZn2O4 in the TiO2-ZnO system was applied as ETL for the device, a high PCE can be achieved, due to its the suitable energy levels and band gap [3]. (3) The compact Ru-doped TiO2 films also have been employed as ETLs for perovskite solar cells.The application of Ru-doped TiO2 films leads to an increase in recombination resistance and a decrease in selective contact resistance[4]. Our studies demonstrated that exploring the high-performance ETL material is an effective approach to improve the PCE of the perovskite-based devices.

A01-PO-18

Plant-Mediated Synthesis of Nano-Silver with Ultrasonic Assisted

Zhen Yuan*, Yimin Wang, Hai Liu, Yihu Ke, Hua Liu
North Minzu University

As a kind of nanomaterials, nano-silver has excellent properties and has been widely used in many fields. The preparation of nano-silver particles by plant-mediated has the characteristics of green, economic and environmental protection, which has been favored by scientists worldwide. Because of its unique cavitation effect and chemical effect, ultrasonic wave is widely used in various reactions. In this experiment, plant-mediated synthesis of nano-silver with ultrasonic assisted was studied systematically.

Cacumen Platycladi(CP) used as the research object. First of all, compared with the normal extraction method, we studied the effect of ultrasound on the extraction of CP. Then, compared with the normal rection of plant-mediated synthesis of nano-silver, the effect of ultrasound on the reaction was studied. Finally, ultrasonic power, silver ion concentration, CP's biomass concentration was respectively studied to ascertain the influence on the preparation of nano-silver.

Through the experiment, ultrasonic wave could improve the extraction efficiency of CP and had no obvious effect on the properties of the biomass. What's more, the production yield of silver nanoparticles can be improved by ultrasonic assisted, and smaller particle size can be prepared. In addition, the increase of ultrasonic power, silver ion concentration and CP' biomass concentration can promote the yield of silver nanoparticles，and the control regulation of silver nanoparticles' diameter is obvious.

Therefore, ultrasonic assisted plant-mediated synthesis can produce nano-silver with controllable particle size, this will provide a new idea for the preparation of precious metal nanomaterials, which is a very promising method.

Keywords: plant-mediated, nano-silver, ultrasonic