WELCOME TO EEMD 2015

EEMD2015 is jointly organized by the annual "International Workshop on Emerging Electronic Materials and Devices" and the annual "International Workshop on Nanomaterials and Nanodevices". EEMD2015 aims at scholarly exchange of information on recent progresses in functional materials and their applications to emerging devices, and at fostering research collaborations.

The week-long EEMD2015 Workshop has two parts: a 3-day conference and a 4-day hands-on training. The conference is from June 30 to July 2, with internationally renowned speakers presenting latest and exciting work. The topics of the conference cover experiment, theory and modeling. The second part of EEMD2015 is a 4-day hands-on training session, July 3 to July 6. The goal of the hands-on session is to help young researchers and students to improve basic research skills by using most advanced modeling techniques and softwares in density functional theory (DFT) for materials modeling and nonequilibrium Green's function (NEGF) based DFT for quantum transport modeling. The hands-on session will also briefly cover theoretical backgrounds of both DFT and NEGF-DFT, and discuss interesting directions for solving emerging problems in materials and devices.

Wish you a wonderful trip in Beijing!

COMMITTEES

Conference Chairpersons

Hongjun Gao vice director of the IOP and the UCAS, China
Hong Guo McGill University, Canada

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Sokrates T. Pantelides Vanderbilt University, USA
Min Ouyang Maryland University, USA
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Scientific Program

June 30, 2015. M234, IOP, CAS	
8:30-10:00	**Session 1** *Chair:* **Werner Hofer**
8:30-8:40	**Opening speeches** **Prof. Hongjun Gao (vice director of IOP , UCAS)** **Prof. Hong Guo (McGill University, Canada)**
8:40-9:30	**Andrea C. Ferrari** *(University of Cambridge, UK)* "Advances in Raman Spectroscopy of Graphene and Layered Materials"
9:30-9:45	**Photo at the front door of Building M, IOP.**
9:45-10:00	**Coffee Break**

10:00-13:30	**Session 2** *Chair:* **Siu Wai Chan**
10:00-10:50	**Andreas Heinrich** *(Almaden Research Center, IBM, USA)* "The Quantum Properties of Magnetic Atoms on Surfaces"
10:50-11:40	**Ludwig Bartels** *(University of California, USA)* "Transition Metal Dichalcogenides: Growth, Characterization and Modification"
11:40-12:10	**Wenjie Liang** *(Institute of Physics, CAS, China)* "Transport Through 1-Dimension Nanostructures"
12:10-13:30	**Lunch time** (2nd floor of the IOP Canteen)

13:30-15:30	**Session 3** *Chair:* **Jiandi Zhang**
13:30-14:20	**Werner Hofer** *(Newcastle University, UK)* TBD
14:20-15:10	**Yu –Hui Tang** (*National Central University, Jhong-Li*) "Spin Torque Effect in Spin-Filter Based Magnetic Tunnel Junction"

15:30-	**Departure from the IOP to UCAS.** ONLY No. 1 bus takes a roundabout way to the Jada Palace Hotel to get luggage. Participants who live there may check your luggage at the hotel registration desk when you check out that morning. Other participants must take your luggage to the conference hall. For safety, we will lock the luggage in a separate room until all the talks of the day have finished.
18:30	**Banquet**

July 1, 2015. International Center, UCAS	
8:00-10:00	**Session 1** *Chair:* **Peter Varga**
8:00-8:50	**Sokrates T. Pantelides** *(Vanderbilt University, USA)* "Things Strange and Wonderful at the Nanoscale"
8:50-9:40	**Thomas Jung** *(Paul Scherrer Institute, Switzerland)* "Supramolecular Materials for Future Devices: Investigating Structure, Electron and Spin States"
9:40-10:00	**Coffee break**

10:00-11:40	**Session 2** *Chair:* **Zheng Gai**
10:00-10:50	**Shouheng Sun** *(Brown University, USA)* "Synthesis and Assembly of Nanoparticle Catalysts for Efficient Electrochemical Reduction Reactions"
10:50-11:40	**Christian Teichert** *(Montanuniversität Leoben, Austria)* "Growth of Small Organic Molecules on a Variety of Graphene Substrates"
12:00-14:00	**Lunch time & Rest**

14:00-16:00	**Session 3** *Chair:* **Zhigang Shuai**
14:00-14:50	**Min Ouyang** *(University of Maryland, USA)* "Quantum Spin Control by Light"

14:50-15:40	**Xudong Xiao** *(Chinese University of Hongkong, China)* “Copper-Based Chalcogenide Compound Semiconductors for Photovoltaic Applications”
15:40-16:00	**Coffee break**

16:00-17:40	**Session 4** *Chair:* **Jing Tao**
16:00-16:50	**Zhigang Shuai** *(Tsinghua University, China)* “Modeling Electron-Phonon Couplings in Organic Thermoelectric Materials”
16:50-17:40	**Xiaogang Peng** *(Zhejiang University, China)* “Control of Photo- and Electro-Generated Excited States of Colloidal Quantum Dots”
18:00-19:00	**Dinner time**
19:00-22:00	**Poster Session**

July 2, 2015. International Center, UCAS

8:00-10:00	**Session 1** *Chair:* **Christian A. Bobisch**
8:00-8:50	**Chonglin Chen** *(University of Texas, San Antonio, USA)* “Interface Mechanical Strain Driven Atomic Layer-by-Layer Oxygen Vacancy Exchange Diffusion”
8:50-9:40	**Peter Varga** *(Vienna University of Technology, Austria)* “Ion-Beam Induced Magnetic Nanostructures”
9:40-10:00	**Coffee break**

10:00-11:40	**Session 2** *Chair:* **Xudong Xiao**
10:00-10:50	**Vladimir Fal’ko** *(University of Manchester, UK)* “Bright, Dark and Semi-dark Excitons and Trions in Transition Metal Dichalcogenides”

10:50-11:40	**Thomas Greber** *(University of Zurich, Switzerland)* "Lateral Segregation on the Nanometer Scale"
12:00-14:00	**Lunch time & Rest**

14:00-15:40	**Session 3** *Chair:* **Karl-Heinz Ernst**
14:00-14:50	**Xiaolong Yang** *(Kunshan New Flat Panel Display Technology Center, China)* "Technology Developments and Challenges in Flexible AMOLED Display"
14:50-15:20	**Yeliang Wang** *(Institute of Physics, CAS, China)* "Epitaxial 2D Materials: Silicene, Germanene, Hafnene and $PtSe_2$"
15:20-15:40	**Coffee break**

15:40-17:30	**Session 4** *Chair:* **Chonglin Chen**
15:40-16:10	**Jianjun Zhang** *(Institute of Physics, CAS, China)* "Shedding Light on SiGe Nanostructures"
16:10-16:40	**Wende Xiao** *(Institute of Physics, CAS, China)* "Controlling the Structural and Spin Properties of Magnetic Metal-Phthalocyanines on Au(111)"
16:40-17:10	**Yunfei Du** *(National Supercomputing Center in Guangzhou)* "Scaling Applications from Six application Domains on Tianhe-2"
17:10-17:30	**Best Poster Awards & Closing Speech: Prof. Sokrates T. Pantelides**
18:00-	**Dinner time**

Abstract

Advances in Raman Spectroscopy of Graphene and Layered Materials

Andrea C. Ferrari

Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 OFA, UK

Raman spectroscopy is an integral part of graphene research [1]. It is used to determine the number and orientation of layers, the quality and types of edges, and the effects of perturbations, such as electric and magnetic fields, strain, doping, disorder and functional groups[2,3]. I will review the state of the art, future directions and open questions in Raman spectroscopy of graphene and related materials, focussing on the effect of disorder[3,4], doping[5,6] and deep UV laser excitation[7]. I will then consider the shear [8] and layer breathing modes(LBMs)[9], due to relative motions of the plane, either perpendicular or parallel to their normal. These modes are present in all layered materials[10,11]. Their detection allows one to directly probe the interlayer interactios [10,11]. They can also be used to determine the elastic constants associated with these displacements: the shear and out-of-plane elastic moduli[12]. This paves the way to the use of Raman spectroscopy to uncover the interface coupling of two-dimensional hybrids and heterostructures[10-12].

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The Quantum Properties of Magnetic Atoms on Surfaces

Andreas Joachim Heinrich

Almaden Research Center, IBM, USA

The scanning tunneling microscope is an amazing experimental tool because of its atomic-scale spatial resolution. This can be combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with microvolt energy resolution. In this talk I will apply these techniques to the investigation of the quantum spin properties of transition metal atoms on surfaces. I will highlight the interesting similarities and differences of those systems with the corresponding gas-phase atoms.

Transition Metal Dichalcogenides: Growth, Characterization and Modification

Ludwig Bartels

University of California at Riverside

I will present the growth of transition metal dichalcogenides films (MoS_2, $MoSe_2$, WS_2, WSe_2, $MoTe_2$) and their alloys via chemical vapor deposition and high vacuum techniques.[4] Local optical spectroscopy in conjunction with photoelectron spectroscopy shed light on the materials' native electronic properties and their variation in the presence of contacts.[1, 2] Post-growth processing allows chalcogen exchange towards local change of bandgap.[3] Deposition onto functional substrates such as ferroelectrics permits further local modification of the material properties toward device applications.[5]

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Transport through 1-dimension Nanostructures

Wenjie Liang, Wengang Lv, Yuchun Zhang, Xiao Guo, Liyan Zhou, Shangqian Zhao

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Ballistic transport and quantum confinements in low dimensional materials play important roles determining many interesting transport behaviors. In this talk we will discuss our progress in studying 1-dimension transport through single double-layered carbon nanotubes and gold nanowires. The interplay between the layered-structure of the former and ballistic transport of electrons in gold will be shown in details.

Spin Torque Effect in Spin-Filter Based Magnetic Tunnel Junction

Yu-Hui Tang(唐毓慧)[1] , *Fa-Chieh Chu(朱法杰)*[1] , *and Nicholas Kioussis*[2]

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Recent discoveries in the ferromagnet/insulator/ferromagnet (FM/I/FM) magnetic tunnel junctions (MTJs) have demonstrated that the relative orientation of the two FM electrodes can be either altered by an external magnetic field, i.e. the tunneling magnetoresistance (TMR) effect, or controlled by a spin-polarized current, i.e. the current-induced magnetization reversal via the spin transfer torque (STT) effect. The spin-transfer, $T_{||}$, and field-like, $T_{\perp}$, components of the STT originate from different components of the spin current accumulated at the FM/I interface and can be expressed in terms of the interplay of spin current densities and of the non-equilibrium interlayer exchange couplings [1], respectively, solely in collinear configurations.

The insulator in conventional FM/I/FM MTJs plays only a passive role in the spin-polarized transport. The evolution beyond passive components has broadened the quest for multifunctional spintronic devices consisting of spin-filter (SF) barriers [2], which exploits the separation of the barrier heights of the two spin channels that can be in turn tuned via an external magnetic field.

In this study [5], the tight binding calculations and the non-equilibrium Green's function formalism is employed to study the effect of the SF-barrier magnetization on the bias behavior of both components of STT in noncollinear FM/I/SF/I/FM junctions. We predict a giant $T_{\perp}$ in contrast to conventional FM/I/FM junctions, which has linear bias dependence, is independent of the SF thickness, and has sign reversal via magnetic field switching. Our results suggest that the novel dual manipulation of $T_\perp$ either by a magnetic field or bias can be employed for "reading" or "writing" processes, respectively, in the next-generation field-like-spin-torque MRAM (FLST-MRAMs). Finally, our newly derived general expressions of noncollinear $T_{||}$ and $T_\perp$ allows the efficient calculation of the STT from collinear ab initio electronic structure calculations [3,4]. (Contract No. NSC 102-2112-M-008-004-MY3)

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Things Strange and Wonderful at the Nanoscale

Sokrates T. Pantelides

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The combination of density functional theory calculations and aberration-corrected scanning transmission electron microscopy is a powerful way to probe nanostructures with atomic resolution. In this talk I will describe a few recent examples: a) the discovery of a new form of crystalline order that we termed "interlaced crystals", namely ABX_2 tetrahedrally-bonded structures in which the two cations that share a sublattice can exist in a large number of ordered arrangements, giving rise to interlaced domains, while the underlying Bravais remains intact [1]; b) fabrication and characterization of ultrathin (three atoms across) nanowires out of a molybdenum dichalcogenide monolayers [2], and c) the demonstration of low-loss electron-energy-loss spectroscopy as a powerful complement to optical spectroscopies, but with spatial resolution [3].

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Supramolecular Materials for Future Devices: Investigating Structure, Electron and Spin States

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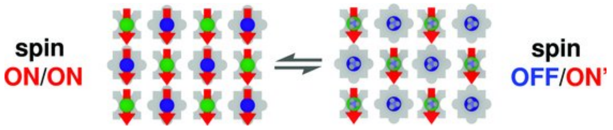
Well defined electronic and spintronic interfaces can be architectured by combining self-assembly and surface science. The atomically clean metal surface in the ultra-high vacuum provides a very specific environment affecting the behaviour of the ad-molecules as well as the adsorbent-adsorbate interaction. Depending on the bonding at the interface, complex electronic and magnetic interactions can occur which can be explored by spectro-microscopy correlation, in this case photoemission and X-ray photoabsorption spectroscopy (PES, XAS) and scanning tunnelling microscopy (STM).

The emergence of quantum dot states from the interaction of a porous network with the 2D (Shockley) surface state of Cu(111) exhibits sufficient residual coupling to show the onset of a band-like structure in angle resolved photoemission [1]. Selected surface-supported molecules have been shown to exhibit ferromagnetic [2] or anti-ferromagnetic [3] exchange interaction, and their spin systems have been shown to be tunable by physical parameters and / or chemical stimuli [4]. Supramolecular chemistry can be combined with on-surface coordination chemistry to reversibly switch the spin of self-assembled bi-molecular arrays [5].

All these examples have in common that the substrate-molecular interfaces are well defined by their production from atomically clean substrates and molecular building blocks. The physics and chemistry of these unprecedented systems, which are addressable by scanning probes, provide insight into novel materials in their assembly, their electronic and spintronic properties which emerge from the interaction of their components down to the scale of single atoms, molecules and bonds.



Scheme 1: Controlling the spin state of a supra-molecular array

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[6] For a complete list of contributing authors refer to the individual publications

Synthesis and Assembly of Nanoparticle Catalysts for Efficient Electrochemical Reduction Reactions

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Recent advance in nano-fabrication has made it possible to design and synthesize nanoparticles with nearly precise controls of nanoparticle size, shape, composition and structure for catalytic applications. In this talk, I will summarize the common methods we used to synthesize monodisperse nanoparticles, especially intermetallic nanoparticles, core/shell nanoparticles, nanowires and their self-assemblies on graphene (or N-doped graphene) surface. I will use Au-, Pt-, and Cu-based elemental and alloy nanoparticles as examples to demonstrate the rational tuning and enhancement of nanoparticle catalysis for selective electrochemical reduction of proton, oxygen, and carbon dioxide for renewable energy applications.

Growth of Small Organic Molecules on A Variety of Graphene Substrates

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Crystalline films of small semiconducting organic molecules offer attractive potential for optoelectronic applications on flexible substrates. However, these applications require a transparent and flexible electrode material; and here the novel material graphene (Gr) comes into play. Since small conjugated molecules like the rod-like molecule para-hexaphenyl (6P) fit well to the hexagonal structure of graphene, growth of 6P on Gr can be expected in a lying configuration.

As observed in situ by low-energy electron microscopy, 6P grows at 240 K indeed in a layer-by-layer mode with lying molecular orientation on Ir(111) supported graphene [1]. 6P islands nucleate at Gr wrinkles [2]. At higher temperatures, needle-like 6P crystallites - also composed of lying molecules - are found [3]. On exfoliated, wrinkle-free graphene, such needles develop with discrete orientations defined by the Gr lattice as detected by atomic-force microscopy [4]. Interestingly, for few-layer exfoliated Gr the needle length decreases significantly with increasing layer number [5].

6P growth can also be used to sense the cleanliness of large-scale, chemical vapor deposited graphene which is transferred by polymethylmethacrylate (PMMA) to the support [6]. There, the increasing length of the resulting 6P needles indicates a reduction of PMMA contaminations of the substrate with increased annealing temperature in hydrogen atmosphere.

Work has been performed in collaboration with M. Kratzer, G. Hlawacek, A. Nevosad, C. Ganser, S. Klima, B. Kaufmann, J. Genser (all Univ. of Leoben), F. Khokhar, R. van Gastl, B. Poelsema, H. Zandvliet University of Twente, Enschede, NL, B. Vasić, A. Matković, U. Ralević, R. Gajić (University of Belgrade), B. C. Bayer, P. R. Kidambi, A. Cabrero-Vilatela, Robert S. Weatherup, S. Hofmann (University of Cambridge, UK), and T. Lelaidier, O. Siri, C. Becker (CINaM, Aix Marseille Université, France).

References:

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Quantum Spin Control by Light

Min Ouyang

University of Maryland – College Park

In this talk a few recent progresses from my group on topic of measurement and control of spin dynamics in various nanostructures will be discussed. In particular, optical technique is employed as a unique tool for spin dynamics measurements with high temporal resolution and sensitivity. By combining ultrafast techniques with nanostructural engineering, different exotic spin-related phenomena can be achieved, including spin manipulation and spin echo, that will also be covered in the talk.

Copper-based Chalcogenide Compound Semiconductors for Photovoltaic Applications

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In the 21st century, we are facing increasingly serious challenges in energy and environment. As a mature technology photovoltaic solar electricity is a perfect solution to meet these challenges. The successful deployment of solar electricity will not only overcome the energy and environment crisis but also sustain a healthy economic and civilizational development.

In photovoltaic technology, production cost is the one of the most important issues that impedes its global-scale application today. In this talk, I will present two copper-based chalcogenide compound semiconductors, the well-known CuInGaSe2 (CIGS) and the emerging Cu2ZnSnS4 (CZTS), as photovoltaic absorber materials that can reduce production cost. Through the discussion on their crystal structures, electronic properties of grain and grain boundary, and device structure and fabrication, I will demonstrate the advantages for their adaption in photovoltaic application. While already successful, the current challenges faced by the CIGS technology and its large-scale application will be addressed. The present status and the challenges for the emerging CZTS will also be presented. In the end, the possibility to hybrid CIGS with the emerging perovskite solar cell technology will also be discussed.

Modelling Electron-Phonon Couplings in Organic Thermoelectric Materials

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The efficiency of a thermoelectric device relies on a dimensionless material parameter, which is known as the thermoelectric figure of merit zT = $S^2\sigma T/\kappa$ with S, σ, κ, and T being respectively the thermopower, the electrical conductivity, the thermal conductivity, and the absolute temperature. Organic electronic materials have been suggested for thermoelectric applications because of their relatively low lattice thermal conductivity. During the past years, significant progress has been made in developing computational schemes to predict the thermoelectric figure of merit at the first-principles level, based on the Boltzmann transport theory [1]. To solve the Boltzmann transport equation, the relaxation time approximation is often invoked and supplied as an empirical parameter. In intrinsic semiconductors, charge carrier scatterings are dominated by phonon scatterings. To calculate the scattering time, we adopted the deformation potential theory to describe the electron-acoustic phonon couplings in the long wavelength limit, and predicted the thermoelectric transport properties of organic semiconductors, such as phthalocyanines [2] and 2,7-dialkyl[1]benzothieno[3,2-b][1]benzothiophene derivatives [3]. Recently, we have gone beyond the simple deformation potential approximation and applied the density functional perturbation theory and Wannier interpolation technique to explicitly consider scatterings from all phonon modes and account for phonon dispersions [4]. As a demonstration, we applied the approach to investigate the charge transport in graphyne nanosheets. We found that electron-phonon scatterings in these two-dimensional carbon materials are dominated by low-energy longitudinal-acoustic phonon scatterings over a wide range of temperatures. The modeling of electron-phonon couplings at the first-principles level can be easily incorporated into the evaluation of thermoelectric properties of interested systems.

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Control of Photo- and Electro-generated Excited States of Colloidal Quantum Dots

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Size-dependent properties of colloidal nanocrystals make them as interesting functional materials. Their solution processibility further enable them as inexpensive and flexible building blocks for devices. Among them, applications of colloidal semiconductor nanocrystals (quantum dots) as photo- and electro-excited emitters are most promising and may impact many industrial sectors. Both photoluminescence and electroluminescence are based on generation and relaxation of the excited states. Thus, properties of excited states should be the key for design, synthesis, understanding, and applications of emitters. Specifically, as promising emissive materials, colloidal quantum dots rely heavily on their excited-state properties, instead of solely the ground-state properties.

The first issue is the design and synthesis of the quantum dots emitters. Limited knowledge on crystallization challenges scientists in the field to develop broadly applicable yet environmentally benign synthesis of colloidal nanocrystals. Their size-dependent properties implies that control of size, shape, size/shape distribution is the baseline for their synthetic chemistry. After ~20 years of efforts, the size dependent optical properties of quantum dots can be controlled at a basic level. Control of the excited states, however, has largely been ignored. This talk shall first discuss synthetic control of the excited states of quantum dots, including possible monitoring tools, identification of hole and electron traps, and the relationship between synthetic conditions and the excited-state properties.

Electroluminescence is mostly realized in solid state, typically in the form of light-emitting-diodes. The second part of the talk shall discuss the advantages of quantum dots light-emitting-diodes. The main focus shall be the electro-generated excited states, including their unique photo-physical properties, outstanding photo-chemical stability, and solution processibility.

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Interface Mechanical Strain Driven Atomic Layer-by-Layer Oxygen Vacancy Exchange Diffusion

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The oxygen vacancy exchange diffusion with oxygen and hydrogen were discovered in the single crystalline $LnBaCo_2O_{5.5}$ (LnBCO, Ln = Er, Pr; 0.0 <   < 0.5) epitaxial films, which paves a new avenue in the development of ultrasensitive chemical nanosensors, energy harvest devices, and many others. Our previous researches indicate that the oxygen vacancy diffuses in the films with oxygen and hydrogen by taking the atomic layer by layer exchange diffusion mechanism. This unprecedented oscillation phenomenon provides the first direct experimental evidence that oxygen/hydrogen atoms diffuse through the LnBCO thin films layer by layer via the oxygen-vacancy-exchange mechanism. It is found that the layer-by-layer oxygen/hydrogen exchange diffusion with oxygen vacancy is highly related to the interface mechanical strain. By examining how the interface strain affects their resistance R under the flow of redox gases, the function of resistance R(T) with temperature T obtained at the saturation reduction under H_2 has a bell shape with maximum at a critical temperature, which increases with increasing the interface strain from a compressive to a tensile one. This indicates that the reduction consists of a reversible adsorption of molecular H_2 followed by a dissociation of H_2, and the dissociated H atoms form OH bonds. The excellent chemical dynamics and ultrafast layer-by-layer oxygen vacancy exchange diffusion suggest that the as-grown LnBCO can be an excellent candidate for energy harvest and chemical sensor developments.

Ion-beam Induced Magnetic Nanostructures

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We demonstrate fabrication of nanoscale magnetic patterns by ion irradiation. For this purpose, we have grown face-centered cubic (fcc) 8-ML, 22ML and 40ML thick Fe films on a Cu(100) single crystal. Since Fe films with a thickness of more than 10ML transform from fcc into bcc, the fcc structure of the 22Ml thick layer was stabilized by growing Fe at a CO pressure of about 10-9 mbar [1] and for the 40ML thick layer co-evaporation of Ni (about 15%) stabilized the fcc structure. A structural transformation of these films from the paramagnetic fcc to the ferromagnetic bcc phase can be induced by ion bombardment [2]. Scanning tunneling microscopy (STM) images show the nucleation of bcc crystallites, which grow with increasing ion dose and eventually result in complete transformation of the film to bcc. Surface magneto-optic Kerr effect (SMOKE) measurements confirm the transformation of the Fe film from paramagnetic to ferromagnetic with in-plane easy axis. Nano-patterning was conducted on these films in situ of the STM via a SiN mask having 80-nm diameter holes to show that the area of transformation is restricted to the irradiated area [3]. We also demonstrated that the transformation of films is possible if they are coated with 2nm Au to protect them from oxidation at ambient conditions. On these “metastable” fcc films various patterns with nm up to m size were produced by ion beam lithography [4] and focused ion beam (FIB) respectively. They were measured by magnetic force microscope (MFM) and by Kerr microscope to see the lower limit of nanostructures possible at the one hand and to see the evaluation of magnetic domains with increasing size on the other hand [5]. Recently we managed to grow such metastable fcc Fe films also on Cu thin films which were grown on Hydrogen stabilized Si(100) substrates.

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Bright, Dark and Semi-Dark Excitons and Trions in Transition Metal Dichalcogenides

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We classify dark and bright states of charged and neutral excitons in two-dimensional (2D) metal dichalcogenides MoX_2 and WX_2 ($X = S$, Se) and analyse their appearance in the optical spectra affected by the inverted sign of spin-orbit splitting of conduction band states in MoX_2 and WX_2. We use diffusion Monte Carlo approach to evaluate the trion binding energy and we determine interpolation formulae for the exciton and trion binding energies to describe their dependence on the 2D lattice screening parameter, the electron/hole band masses, and electron-hole exchange.

Lateral Segregation on the Nanometer Scale

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Surface segregation causes the deviation of a multicomponent system from the bulk composition. For intermetallic compounds it has e.g. implications in hydrogen storage [1] or nanocatalysis [2]. Normally, surface segregation proceeds perpendicular to the surface. The driving forces for segregation are strain release and surface energy minimization [3]. However, it also depends on adsorbates, which e.g. leads in chemical waves to segregation parallel to the surface [4]. Here we report on lateral segregation in the top layer of a PtRh (111) surface on the nanometer scale [5]. This is obtained during the growth of a single layer of hexagonal boron nitride on the (111) surface of a PtRh crystal. The investigation of h-BN/PtRh(111) reveals a corrugated super-honeycomb, with 11 hBN units on top of 10 primitive substrate unit cells. Lateral segregation occurs in the topmost layer of the substrate during growth of h-BN, where Rh atoms must form islands where nitrogen sits on top of the substrate atoms. This picture is drawn from x-ray photoelectron spectroscopy (XPS) and x-ray photoelectron diffraction (XPD) data.

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Technology Developments and Challenges in Flexible AMOLED Display

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From CRT (Cathode Ray Tube) to FPD (Flat Panel Display), display technology always presents the development tedency of portability and flexibility. Especially in the past three years, more attention has been focused on the flexible AMOLED display for its potential applications to cellular, automobile and TV markets ect. For display industry the technical development in flexible display may include three main stages: bendable, foldable and deformable. Although it’s still under the bendable stage, recent flexible display products in cellphone and TV have already been published, indicating a very promising and bright future for flexible display.

However, before flexible display techniques can be transferred from pilot line to mass production, many challenges have to be solved such as material, processibility, stability and reliability issues. First, new materials (such as polymer) will be introduced to replace the rigid substrate, acting as the flexible substrate. Besides, the fabrication processes towards flexible display have to be tuned and optimized to meet requirements of performance, cost, and new material compatibility as well. Flexible display device also may suffer from the excessive bending, leading to the device fatigue issue caused by unbalanced stresses within the material layers. Finally, the device lifetime is directly related to the device TFE (Thin Film Encapsulation) quality. This is because that pending on the protective film thickness and structure, oxygen and water may penetrate the protective films, damage the OLED materials and compromise the device performances as a result.

Epitaxial 2D Materials: Silicene, Germanene, Hafnene and PtSe2

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The novel properties of graphene honeycomb structure have spurred tremendous interest in investigating other two-dimensional (2D) layered structures beyond graphene. In this talk, I will report the fabrication and properties of several graphene-like materials, such as, silicene[1], germanene[2] and hafnene[3], wherein silicon (germanium or hafnium) atoms are substituted for carbon atoms in graphene. A new semiconducting transition-metal-dichalcogenide, monolayer $PtSe_2$[4], grown by direct selenization of Pt will also be introduced. Molecular beam epitaxial (MBE) growth technique is used to form large-scale single-crystalline materials on solid surfaces. In addition, the stacking heterolayers based on several these kinds of 2D materials will be also presented. We expect that these materials will show intriguing physical property and promising potential applications in nanoscale devices.

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*In collaboration with Prof. Zhi-hui QIN from Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences for germanene work. Yao Wei and Prof. Shu-yun Zhou from Tsinghua University for ARPES; Dr. Chen Li from Oak Ridge National Laboratory and Prof. S. Penneycook from National University of Singapore for STEM; Xiao Ren and Prof. Hai-tao Yang from Institute of Physics for photocatalysis experiment; Shiru Song, Dr. Jiatao Sun, Dr.Yuyang Zhang and Prof. Shixuan Du from Institute of Physics for theoretic calculations; Prof. Sokrates Pantelides from Vanderbilt University and Prof. Min Ouyang from University of Maryland for data analysis and constructive suggestions.

Shedding Light on SiGe Nanostructures

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Ge nanostructures on Si(001) are interesting not only for understanding fundamental properties of heteroepitaxial growth but also for their applications in electronic and thermoelectric devices. Firstly, I will talk about the site-controlled growth of ordered SiGe islands and the first demonstrated devices with tensile strained Si channel on top of buried SiGe islands with enhanced electron mobility. Secondly, I will report on a new method to directly and horizontally grow micron-long Ge nanowires on Si(001) with a height of only 3 unit cells. First transistor-type devices made from single wires show low-resistive electrical contacts and single hole transport. Such Ge wires hold promise for observing exotic quantum states, like Majorana fermions, and provide a new development route for silicon-based nanoelectronics. Lastly, I will show you novel 1D Ge nanostructures, such as nanowire bundles, dumbbells, matchsticks and dot chains, observed by carefully tuning the strain fields.

Controlling the Structural and Spin Properties of Magnetic Metal-Phthalocyanines on Au(111)

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Metal-phthalocyanines (MPc) and their derives have attracted increasing interest in recent years, due to their potential applications in molecular electronics, spintronics, sensors and so on. To this end, it is essential to tune the structural electronic and spin properties of MPcs. Using low-temperature scanning tunneling microscopy (LT-STM), we demonstrate that the structural and spin properties of MnPc on Au(111) surface can be tuned by hydrogen atoms. STM experiments and density functional theory (DFT) calculations reveal that the molecular spin decreases from S=3/2 to S=1 and the molecule-substrate coupling weakens after adsorption of a hydrogen atom on a MnPc molecule, leading to the quenching of Kondo effect at 4.2 K. The molecular spin and Kondo effect can be recovered by local voltage pulse or sample heating. Moreover, we observe site-dependent g-factor of a single dehydrogenated MnPc molecules on Au(111). This is achieved by exploring the magnetic-field dependence of the extended Kondo effect at different atomic sites of the molecule. Importantly, an inhomogeneous distribution of the g-factor inside a single molecule was revealed. Our results open up a new route to controal local spin properties within a single molecule, which opens up new avenue of broader applications based on molecular electronic and spin states.

Scaling Applications from Six Application Domains on Tianhe-2

Yufei Du （杜云飞）

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The National Supercomputer Center in Guangzhou (NSCC-GZ) undertakes interdisciplinary research on high-performance and cloud computing and big data analysis. It hosts the Milky Way II (Tianhe-II) supercomputer combining Intel Xeon processors and Xeon Phi (MIC) coprocessors, and rated fastest in the world by the TOP500 since June 2013. NSCC-GZ serves six application domains: Earth science and environmental engineering, materials science and engineering, life sciences and personalised medicine, digital design and manufacturing, energy and related technologies, and smart city. This report focuses on the development of these six application domains over the last year.

Yunfei Du received his doctor degree from National University of Defense Technology, China in 2008. His research interests focus on parallel and distributed systems, fault tolerance, and scientific computing. He is the chief engineer of National Supercomputing Center in Guangzhou now.

Abstract
of
Poster

Conditions for Quantized Anisotropic Magnetoresistance

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Anisotropic magnetoresistance (AMR) is a phenomenon that the resistivity of a ferromagnet depends on the angle θ between the electric current and the magnetization direction.The traditional AMR in bulk shows the continuous variation with simple cos2θ shape. When the length of a conductor reduces to less than the mean free path of the electrons, the ballistic transport occurs. The first study[1]on the AMR in ballistic regime was done byJ. Velev et al,predicting a novel quantized stepwise θ-dependence of the conductance (quantized AMR, or QAMR). However in most latter experiments, the QAMR character disappears. Thus, the conditions for emerging the QAMR are crucial but lacking.

We use the NANODCAL package based on the non-equilibrium Green's function-density functional theory (NEGF-DFT) to study conditions for the appearance of the QAMR, focusing on the role of the spin-orbital interaction (SOI), the effects of the transverse sizes and the temperature respectively[2].Firstly, It has been demonstrated that the SOI is a precondition and the transverse size is a crucial condition for QAMR to emerge. Furthermore, we show for the first timethe evolution of QAMR from a stepwise shape, corresponding to small transverse sizes, to a classical smooth cos2θshape, corresponding to large transverse sizes. In addition, we prove the strong temperature dependence of QAMR, so a low temperature is necessary.

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Quantum Transport Properties of Au/Oligothiophene/Au Single Molecular Junctions: A First-principles Study

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Controlling molecules to create desired transport properties in an electronic nanodevice is a promising way toward nanoelectronics. Lately, we have investigated the conductance switching properties during the stretching of Au/oligothiophene dimethylene dithiol/Au single molecule junctions [1] by the first-principles method with the non-equilibrium Green's function approach, which are in agreement with the experimental measurements and observations [2]. In this study, the first-principles calculation is employed to give a comprehensive understanding of the current-voltage (I-V) characteristics in 3T1DT (with three thiophene rings) and 4T1DT (with four thiophene rings) cases. At the breaking point, the highest occupied molecular orbital (HOMO) of longer 4T1DT is closer to the Fermi energy so that the 4T1DT is more conductive than is the shorter 3T1DT. When the applied bias is nonzero, the transmission peak resulting from the HOMO level is shifted with the chemical potential of right electrode. With discrepant shifting rates of projected density of states(PDOS) of molecule and electrode at the junction break, the I-V curve characters highly asymmetric and stepped characteristics for both cases. Once this transmission peak is included in the bias window, the abrupt enhancement of current can be found at lower (higher) bias for 4T1DT (3T1DT) case.

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Magnetic Property of Fullerene C_{20} : A First-Principles Study

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From the production in the gas phase by Prinzbach[1], the C_{20} as the smallest fullerene has been attracted considerable attention among scientists. In the following year, Wang et al[2]sucessfully synthesized the solid phase of C_{20} using ion beam irradiation method and found that the fullerene C_{20} behave as the building block of hexagonal crystal. In addition, Jo et al. [3] predicted the magnetism in C_{20} cage structure due to its pentagon-bunching structure.

To investigate the underlying mechanism of the magnetism of fullerene C_{20} cage structure, we employed the density functional theory (DFT) within thenonequilibrium Keldysh Green's function (NEGF) formalism to study the spin-polarized density of states of the isolated nonmagnetic C_{60} and C_{20} bowl-like molecules, which are truncated by the mixture of pentagons and hexagons as shown in Figs. 1(a) and (b), and of the isolated magnetic C_{20} cage and C_{15} bowl-like molecules, which exhibit purely pentagon-bunching structure as shown in Figs. 1(c) and (d). For the C_{15} bowl-like structures, the spin-polarized molecular levels are mainly contributed by those C atoms on the zigzag edge, while, for the C_{20} cage structure, all molecular levels are spin-polarized resulting from the ziazag boundaries between pentagons. Such zigzag-boundary induced magnetic properties of C_{20} cage and C_{15} bowl-like molecule can be analog to the graphene nanoribbon with zigzag edges [4]. Moreover, the non-magnetic and insulating properties of C_{60} and C_{20} bowl-like molecules can be attributed to the mixture of zigzag and armchair boundaries between hexagon and pentagons.(Contract No. NSC 102-2112-M-008-004-MY3)

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Structures and Electronic Properties of Phosphorene Grain Boundaries

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Phosphorene grain boundaries were studied by using density functional theory (DFT). The atomic structures and electronic properties were investigated for phosphorene monolayer with grain boundaries of different misorientation angles. The formation energies of grain boundaries can be associated with the misorientation angle. The band gap of phosphorene can be tuned by symmetric grain boundaries. These theoretical results may provide useful insights for the applications of polycrystalline phosphorene materials in micro-electronics and optics.

Vibrational Properties of Rigid-layer Modes in Few-layer Black Phosphorus

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Stacking two-dimensional (2D) materials into multi-layers or heterostructures, known as van der Waals (vdW) epitaxy, is an essential degree of freedom for tuning their properties on demand. Few-layer black phosphorus (FLBP), a material with high potential for nano- and optoelectronics applications, appears to have interlayer couplings much stronger than graphene and other 2D systems. Indeed, these couplings call into question whether the stacking of FLBP can be governed only by vdW interactions, which is of crucial importance for epitaxy and property refinement. Here, we perform a theoretical investigation of the vibrational properties of rigid-layer modes in FLBP, which reflect directly its interlayer coupling. With increasing sample thickness, we find that the vibrational frequencies of rigid layer modes are different from the one-dimensional chain model, especially for the armchair shear mode. Our calculations also show the divergence of interlayer force constants between surface and inner layers. An anomalous phonon-phonon coupling is also found for the armchair shear mode and a low-frequency optical mode. By computing uniaxial stress effects, inter-atomic force constants, and electron densities, we provide a compelling demonstration that these properties are the consequence of strong and highly directional interlayer interactions arising from electronic hybridization of the lone electron-pairs of FLBP, rather than from vdW interactions. This exceptional interlayer coupling mechanism controls the stacking stability of BP layers and thus opens a new avenue beyond vdW epitaxy for understanding the design of 2D heterostructures.

Structure and Stability of Oxidized Epitaxial Graphene by Density Functional Theory Studies

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Graphene oxide (GO) holds great promise for applications in nano-electronics, optics, sensors, and energy storage. Understanding the structure of GO is important to control the properties and hence realize the applications of this material. In this work, we investigated the thermochemical and structural properties of oxidized epitaxial graphene (EGO) films on SiC by density functional theory calculations. Studies show that these EGO films present well-structured carbon layers with uniform thickness, including minimal defects and holes. At room temperature, EGO is metastable -- it undergoes chemical modifications and spontaneous reductions mainly through the formation and desorption of water. This aging process leads to a non-homogenous intralayer structure in EGO consisting of oxidized and unoxidized graphene domains, which enhance both chemical and kinetic stability of the material. The oxidized regions are rich in hydroxyl species and prone to trap water, forming hydrogen bonding network with neighboring layers, and leading to an interlayer spacing up to 9 angstrom.

Coherent Single-Spin Source in 2D TI

Attached paper: Yanxia Xing, Zhong-liu Yang, Qing-feng Sun and Jian Wang, Phys. Rev. B 90, 075435 (2014).

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The proposed single-spin emitter can be an important building block of future spintronic devices.So, we report on an on-demand single-spin source based on the two-dimensional (2D) Topological insulator. Due to the nature of the helical states of the topological insulator, one or several spin pairs can be pumped out per cycle giving rise to a pure quantized alternating spin current by periodically varying the gate voltages of two quantum dots that are connected to a 2D topological insulator via tunneling barriers. Depending on the phase difference between two gate voltages, this device can serve as an on-demand single-spin emitter or single-charge emitter. Again, due to the helicity of the topological insulator, the single-spin emitter or charge emitter is dissipationless and immune to disorder.

Electronic Properties of Armchair Graphene Nanoribbons with BN-doping

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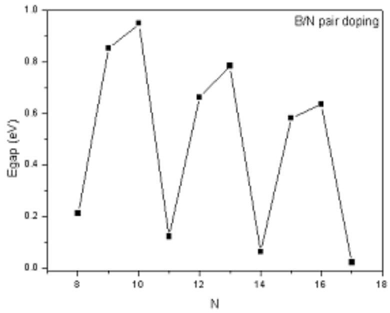
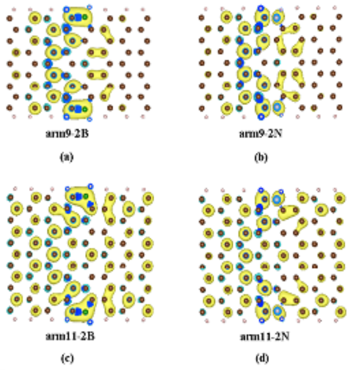
Since 2004, graphene[1-4] has caught the eyes of many scientists due to its novel physical properties. Particularly, graphene nanoribbons (GNRs) [5-9] have attracted much attention for their unique electronic properties including either metallic or semiconducting behavior as a function of ribbon width. GNRs have opened up huge possibilities for electronic device manufacturing. It has been shown that zigzag-edged graphene nanoribbons (ZGNRs) [10,11] and armchair-edged graphene nanoribbons (AGNRs) [12,13] can be used for nanoelectric devices due to their energy gaps. AGNRs are either semiconducting or metallic depending on their width. All GNRs have energy gaps which are inversely proportional to the ribbon width. According to earlier studies [14,15], the electronic properties of AGNRs and the gap openings of the three families of AGNRs ($3n$, $3n^{+1}$, $3n^{+2}$) strongly depend on their ribbon width, where n is an integer. The AGNRs are metallic if the number of rows of carbon is $3n+2$. AGNRs' energy gap appears because of quantum confinement and the crucial effect of the edges. But it is not easy to tune the width of the energy gap of AGNRs smoothly by experimentally varying the ribbon width. Chemical doping has been revealed to be an influential factor in determining the electronic properties of GNRs in nanoscale [16, 17].

Although the electronic structure and transport properties in the presence of impurity have been investigated in both graphene and graphene ribbons, how these properties manifest in AGNRs is still an area which calls for more attention. Recently, it has been found that nitrogen (N) and boron (B) atoms are typical substitutional dopants in carbon materials and that B/N doping at the different sites would lead to changes of electronic properties in GNRs. Density functional theory (DFT) calculations predict energy gap oscillations as a function of the GNR for very small widths. A gapped magnetic ground state has been suggested to be due to an antiferromagnetic interedge superexchange. Liu et al found that armchair BCN-hybrid nanoribbons present magnetism along the edges of the nanoribbons if B and N atoms are unpaired in the nanoribbons. N. Kumar et al investigated the specific configurations of B and N doping in GNRs showing that they exhibit some interesting electronic properties and excellent characteristics for application. However, further theoretical work is still needed to elucidate diverse BN-doping configurations within the AGNRs. Therefore, the influence of the B and N impurity on the spin-dependent electronic properties of AGNRs deserves careful study.

Using the first-principles calculations based on density functional theory, we investigated the electronic properties of armchair graphene nanoribbons (AGNRs) with boron nitrogen (BN) doping. The B and N impurities can adjust the electronic properties of the AGNRs, whose features strongly depend on the impurity types and the ribbon width of the AGNRs. Interestingly, with the increase of the ribbon width, the energy gap of the AGNRs with B/N pair doping is oscillatory. The AGNRs with B or N doping show metallic behavior, and the localized unsaturated electronic states on the edge atoms lead to magnetism. These unconventional doping effects could be used to design semiconductor electronic devices.





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Enhancing Thermoelectric Figure-of-merit by Low-dimensional Electrical Transport in Phonon-glass Crystals

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Low-dimensional electronic and glassy phononic transport are two important ingredients of highly-efficient thermoelectric materials, they come from two branches of the thermoelectric research . One is to control electronic transport in the low dimension, while the other is to apply phonon engineering in the bulk. Recent work has benefited much from combining these two approaches, e.g., phonon engineering in low-dimensional materials. Here, we propose to employ the low dimensional electronic structure in bulk phonon-glass crystal as an alternative way to increase the thermoelectric efficiency. Through first-principles electronic structure calculation and classical Equilibrium molecular dynamics simulation, we show that the pi-pi stacking Bis-Dithienothiophene molecular crystal is a promising candidate for such an approach. This is determined by the nature of its chemical bonding. Without any optimization of the material parameter, we obtain a maximum room-temperature figure of merit, ZT ,of 1.48 at optimal doping, thus validating our idea.

Perfect Spin Filtering Effect and Negative Differential Behavior in Phosphorus-doped Zigzag Graphene Nanoribbons

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On the basis of the density functional theory combined with the Keldysh nonequilibrium Green's function method, we investigate the spin-dependent transport properties of single-edge phosphorus-doped ZGNR systems with different widths. The results show a perfect spin filtering effect reaching 100% at a wide bias range in both P and AP spin configurations for all systems, especially for 6-ZGNR-P system. Instructively, for the AP configuration, the ↓-spin current of the 4-ZGNR-P system appears a negative differential effect. By analyzing transmission spectrum and spin-resolved band structures of the electrode, we elucidate the mechanism for these peculiar properties. Our findings provide a new way to produce multifunctional spin spintronic devices based on phosphorus-doped zigzag graphene nanoribbons.

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Origin of Interfacial Perpendicular Magnetic Anisotropy in MgO/CoFe/metallic Capping Layer Structures

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Spin-transfer-torque magnetic random access memory (STT-MRAM) attracts extensive attentions due to its non-volatility, high density and low power consumption. The core device in STT-MRAM is CoFeB/MgO-based magnetic tunnel junction (MTJ), which possesses a high tunnel magnetoresistance ratio as well as a large value of perpendicular magnetic anisotropy (PMA). It has been experimentally proven that a capping layer coating on CoFeB layer is essential to obtain a strong PMA. However, the physical mechanism of such effect remains unclear. In this paper, we investigate the origin of the PMA in MgO/CoFe/metallic capping layer structures by using a first-principles computation scheme combined with perturbation theory. The calculated magnetic anisotropy energies agree well with experimental results. We find that interfacial PMA in the three-layer structures comes from both the MgO/CoFe and CoFe/capping layer interfaces, which can be analyzed separately. Furthermore, the PMA in CoFe/capping layer interfaces is attributed to the hybridization between the 3*d* orbitals of interfacial Co and the 4*d* or 5*d* orbitals of capping layer atoms with a strong spin-orbit coupling induced splitting in the PDOS around the Fermi Energy. This work can significantly benefit the research and development of nanoscale STT-MRAM.

Spin/orbital Coupling and Charge Ordering in LaMnO3/SrMnO3 Superlattice

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Coupled spin, orbital and charge ordering in half-doped perovskite $La_{1/2}Sr_{1/2}MnO_3$ (LSMO) superlattice are quantitatively investigated in realspace using the generalized gradient approximation (GGA) plus on-site Coulomb repulsion U (GGA+U) method. It is found that the high spin Mn^{3+} site exhibits an elongation of MnO_6 octahedral for the Jahn-Teller distortion, with estimated distortion energy about 0.1 eV. The occupied e_g states of Mn^{3+} cations are predominantly of d_z^2 character, which contribute mainly to the orbital ordering in LSMO. Mn^{3+} and Mn^{4+} ions show electronic disproportionation and lead to an e_g charge ordering distribution. As the thickness of one period of LSMO superlattice increases, the spin magnetic moments increase and the charge order effect reduces.

Piezoelectric Properties in 2Dtransition metal Dichalcogenide: A First-principles Study

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2 dimensional MoS2is considered to be a good candidate forthe next generation nanoelectronics. Recently the piezoelectric in 2 dimensional MoS_2has been experimentally proofed. This implied its potential application in piezotronics. 2D transition metal dichalcogenide(2D-TMDs)to which MoS2belongsincludean aggregate of a wide range ofmaterials haveMoS2like structure. A first principle studyon the piezoelectric properties of 2D-TMDsis meaningful to develop future piezotronic devices.

In this work, different kinds of monolayer 2D-TMDs including MoS_2,$MoSe_2$, $MoTe_2$, WS_2, WSe_2, $WTe_2$are studied. As wildly known the 2D-TMDs has two phases 2H(non-central-symmetry) and 1T(central-symmetry), and piezoelectric can only exist in the 2Hphase. So, first we calculate the total energy of different kinds of 2D-TMDs mentioned above and their 2H and 1T phases were took in consideration. Then the band structures of the 2H stable ones are calculated to confirm whether they have band gap, because piezoelectric can’t exist in metals. According to the stability and the band structures, the 2Hphasemonolayer MoS_2, WS_2were selected as candidates for piezotronic devices.

Finally we calculate the macroscopic polarization of MoS_2 and WS_2employing the Berry Phase method, then the linear and second order piezoelectric coefficients were given by fitting the polarization-strain curves. The polynomial for fitting is as follows:$P = Psp + e1\varepsilon + e2\varepsilon 2$

Figure 2. Macro polarization-strain relationship in monolayer MoS_2, WS_2. This diagram shows good linear relations.

All of them present excellent linear relationship between polarization and strain. The piezoelectric coefficients are shown in table 1.

This result implies that WS_2can also been applied in piezotronic devices, and further due to WS’s smaller second order piezoelectric coefficients, a piezotronic nano device or a force nano sensor base on WS_2 may present more linear response.

Spin-injection Efficiency and Tunnel Magnetoresistance of the Ni/Monolayer Black Phosphorus/Ni

Trilayer Junctions from First Principles

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We report first principles calculations of nonequilibrium quantum transport properties on the Ni/Monolayer Black Phosphorus(MBP)/Ni trilayer magnetic tunnel junctions (MTJs). The spin-injection efficiency (SIE) and the tunnel magneto resistance (TMR) are studied for two different MTJs in Ni(111)/MBP/Ni(111) and

Ni(100)/MBP/Ni(100) forms. For both MTJs, the SIE is larger when magnetic moments of the two ferro-magnetic Ni layers are in parallel configuration (PC) then when they are in antiparallel configuration (APC). The PC Ni(100)/MBP/Ni(100) junction keeps a higher and constant SIE around 60from 0 to 100 mV, and also shows a stable TMR value around 40Ni(111)/MBP/Ni(111) junction, however, has a drastically decreasing TMR when finite bias is applied. These first principles studies indicate the promising application of the Ni(100)/MBP/Ni(100) trilayer on spintronics devices since it has higher and more stable SIE and TMR values than the Ni(111)/MBP/Ni(111) trilayer has.

Spin Effects on Thermoelectric Properties of B-N Co-Doped Zigzag Graphene Nanoribbons

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Based on the nonequilibrium Green's functions combined with the density functional theory (NGF-DFT), we investigate the transport properties of zigzag graphene nanoribbons (ZGNRs) co-doped with boron (B) and nitrogen (N) atoms. Dopings of III-group B atoms and V-group N atoms are widely used methods to functionalize ZGNRs and manipulate the properties therein. Separately they usually introduce opposite impurity types. In this work, we consider the effects of co-doping these two opposite types of impurities closely on one edge of an otherwise pristine ZGNRs in the ferromagnetic (FM) state. The impurities introduce a transmission dip near the Fermi energy and split the spin-up transmission spectrum slightly from the spin-down one. In this case, the spin Seebeck coefficient S_s is greatly enhanced and can be larger than the charge Seebeck coefficient S_c. For example, as shown in the figure, a strong spin thermopower effect may occurs with $|S_s| \gg |S_c|$ at the room temperature in 4-ZGNRs. The dependence of thermopower on the geometry parameters of the systems and the doping positions are studied in detail.

Coherent Single-Spin Source in 2D TI

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The proposed single-spin emitter can be an important building block of future spintronic devices. So, we report on an on-demand single-spin source based on the two-dimensional (2D) Topological insulator. Due to the nature of the helical states of the topological insulator, one or several spin pairs can be pumped out per cycle giving rise to a pure quantized alternating spin current by periodically varying the gate voltages of two quantum dots that are connected to a 2D topological insulator via tunneling barriers. Depending on the phase difference between two gate voltages, this device can serve as an on-demand single-spin emitter or single-charge emitter. Again, due to the helicity of the topological insulator, the single-spin emitter or charge emitter is dissipationless and immune to disorder.

Impact of Oxide Layer Thickness on Electrical Transport of MIS Diodebased on ZnOnanostructure

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ZnO is widely used in strain sensors, UV detectors, solar cells and so on. Although many experimental studies about MIS diode based on ZnO nanostructure has been published, theoretical simulations on the devices are rare.

In this work, we built a 1D nanostructure modelas illustrated in the right figure. Doping concentration of ZnO is 5x1017cm-3, and left contact is Ohmic. Finite-element simulations were used to solving of the Schrödinger, Poisson equations for the devices, as implemented in Next nano 3 code.

As the barrier height of MgO/Metal is relatively low while the barrier height of Al_2O_3/Metal is high, carrier accumulation regions were observed at ZnO/MgO interfaces and carrier depletion regions were observed at ZnO/Al_2O_3interfaces. Because of major carriers transport, currents in MgO MIS model were determined by tunneling probabilities of both directions rather than delivery rates of carriers, so that current densities decreased rapidly as MgO layer thickness increased. For Al_2O_3MIS model, due to limit of minority carriers delivery rates, current densities in Al_2O_3MIS model with low voltages were very small. The thickness of Al_2O_3modified the lengths of depletion regions, and then changed the effective barrier heights, so that turn-on voltages of Al_2O_3MISmodel increased obviously as Al_2O_3layer thickened. With high voltages, current densities increased monotonously as voltages increasing, and decreased as Al_2O_3layer thickened with same voltages.

The impact of MgO insulating layer is blocking recombination of electrons and holes, and the impact of Al_2O_3insulating layer is changing the effective barrier height.

Spin-resolved Transport Properties in Zigzag α-graphyne Nanoribbons with Symmetric and Asymmetric Edge Fluorinations

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Graphyne, a new kind of carbon allotrope, can be obtained by replacing some carbon-carbon sp^2 bonds in graphene with acetylenic linkages [1]. In 2010, large area films of graphdiyne have been successfully fabricated on copper surface [2], which is a big step towards the preparation of other graphynes. α-graphyne is a zero-gap semiconductor with a direction-dependent Dirac cones [3]. One way to get a band gap is tailoring it into armchair and zigzag nanoribbons, short for AαGYNRs and ZαGYNRs. All AαGYNRs are nonmagnetic with an oscillated band gap [4]. While ZαGYNRs have a stable antiferromagnetic configuration, and the band structure are spin degenerate [4]. Former researches show that the edge states have a significant effect on their electronic and magnetic properties [5], and the transport properties are highly rely on the symmetry of geometric [6]. Therefore, we are mainly centering on the electronic and transport properties of edge symmetric and asymmetric fluorinated ZαGYNRs.

The calculations are based on the non-equilibrium Green’s function method and the spin-polarized density functional theory. Our results show edge fluorination can enhance the stability of ZαGYNRs. The spin-resolved transport calculation reveal that the devices of symmetric fluorinated F-ZαGYNRs-F with odd ribbon widths behave as a conductor with a linear current-voltage relationship, while the semiconductor property and perfect bipolar spin-filtering effect can be observed in those devices with even ribbon widths in antiparallel spin configuration (APC) of two electrodes. In contrast, the spin-resolved transport properties of the asymmetric edge fluorinated F2-ZαGYNRs-F systems are independent of the ribbon width, but influenced largely by the spin configuration of two electrodes. Interestingly, the F2-ZαGYNRs-F can be acted as a multifunctional device with nearly 100% bipolar spin-filtering efficiency, 10^8 order spin rectification ratio and negative differential resistance effect in a wide bias region. The magnetoresistance effect with the order of 10^8% has also been predicted. All these suggest ZαGYNRs with asymmetric edge fluorination can be considered as a promising candidate material for nano-electronics and spintronics.

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First-principles Study on the Electronic Properties of Armchair WSe_2 Nanoribbons

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Keywords: electronic, density functional theory, WSe_2, armchair nanoribbons

Transition metal dichalcogenides (TMDs), a new family of two-dimensional materials with graphene-like structure, are a series of materials with the molecular formula of MX_2 (typically M=Mo/W; X=S/Se). For two-dimensional monolayer, they seem to be semiconducting with a wide electron band gap. However, less attention has been paid to the properties of their nanoribbons. In this work, density functional theory (DFT) as well as non-equilibrium Green's Function (NEGF) method are employed to investigate the electronic transport properties of armchair WSe_2 nanoribbons (AWNR-N, N defines ribbon width). Norm-conserving pseudopotentials are adopted within the local density approximation (LDA) of Perdew-Zunger with energy (charge density) cutoff up to 50 Ry (500 Ry). AWNR-5, -6 -7 without H-passivation and with H-passivation are under investigation. For AWNR without H-passivation, the electronic band gap seems to increases with increasing ribbon width and a metal-semiconductor transition can be discovered. After H-passivation, the band gap of the investigated AWNRs tends to converge with the value of ~1.3 eV, which may be caused by the stabilization of the dangling bonds of the nanoribbon edge.