2009 International Workshop on

Nanostructures & Nanodevices

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July 1-3, 2009

Institute of Physics, Chinese Academy of Sciences, Beijing, China

July 6-7, 2009

Sichuan University, Sichuan, China

Sponsors

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“中科院-国家外专局纳米材料与器件研究国际合作团队”
（北京部分）
International Workshop on Nanomaterials and Nanodevices

(Beijing Session, July 1-3, 2009)

地点 (Venue)： 物理所D楼212报告厅 (IOP Building D 212)

Scientific Program	
July 1, IOP Building D 212	
8: 30	**Opening Ceremony and Welcome Remarks:** Jian Shen *(Oak Ridge National Laboratory, USA)* Hongjun Gao *(Institute of Physics ,CAS)*
8：40－10：20	**Session 1** *Chair: Karl-Heinz Ernst*
8：40－9：20	Andreas J. Heinrich *(Almaden Research Center, IBM)* “Quantum Magnetism of Atoms on Surfaces: an STM Study”
9：20－10：00	W.A. Hofer *(The University of Liverpool, UK)* “Dynamic Processes Observed by Scanning Tunnelling Microscopes: Conformation Changes, Diffusion and Vibrations”
10：00－10：20	Jichun Lian *(PhD student, IOP, CAS)* “Characterization of Point Defects on MgO(001) films”
10：20－10：30	Coffee Break and Photos
10：30－11：50	**Session 2** *Chair: W.A. Hofer*
10：30－11：10	Karl-Heinz Ernst *(Swiss Federal Laboratories for Materials Testing and Research (Empa), Switzerland)* “Symmetry Mismatch and Reversible Polymorphism in Two Dimensional Molecular Crystals”
11：10－11：50	Shuheng Pan *(University of Houston, USA)* “Direct Probe of the Key Building Block of the Fe-based Superconductors with Scanning Tunneling Microscopy/Spectroscopy (STM/S)”
11：50	Lunch (IOP Restaurant)

13：30—15：30	**Session 3** *Chair: Feng Liu*
13：30—14：10	Hong Guo *(Mcgill University, Canada)* "Atomic Simulation of Disorder Effects in Magnetic Tunnel Junctions"
14：10—14：40	Xincheng Xie *(Oklahoma State University, USA/Institute of Physics, CAS, China)* "Dephasing and Disorder Effects in Quantum Spin Hall Effect"
14：40—15：10	Xianggang Qiu *(Institute of Physics, CAS, China)* "Interference Phenomena in Superconducting Nb Thin Films Perforated with Periodic Hole Array"
15：10—15：40	Hongqi Xu *(Lund University, Sweden)* "Spin Physics and Kondo Effect in Semiconductor Quantum Dots "
15：40—16：00	Hao Hu *(PhD student, IOP, CAS)* "Theory of Directed Nucleation of Strained Islands on Patterned Substrates"
16：00—16：10	Coffee Break
16：10—18：00	**Session 4** *Chair: Yi Shi*
16：10—16：40	Jian Shen *(Oak Ridge National Laboratory, USA)* "Emergent Phenomena in Spatially Confined Manganites"
16：40—17：20	Ru Huang *(Peking University)* "Gate-All-Around Silicon Nanowire Transistors from Top-Down Approach: Fabrication and Experimental Characterization"
17：20—18：00	Ming Liu *(Institute of Microelectronics, CAS)* "Nano-crystal Based Charge Trapping Non-Volatile Memory"
18：00	Banquet (Da-Zhai-Men Restaurant)

July 2, IOP Building D 212	
8：30－10：30	**Session 5** *Chair: Shouheng Sun*
8：30－9：10	Hongjie Dai *(Stanford University, USA)* "Carbon Nanotubes and Graphene Nanoribbons"
9：10－9：50	Chunyung Sung *(T. J. Watson Research Center, IBM)* "Post CMOS Nanoelectronics Research for the Next Generation Logic Switches"
9：50－10：30	Siu-Wai Chan *(Columbia University,USA)* "Towards Carbon Based Electronics"
10：30－10：40	Coffee Break
10：40－12：30	**Session 6** *Chair: Hongjie Dai*
10：40－11：10	Shouheng Sun *(Brown University, USA)* "Functional Nanoparticles: Synthesis and Potential Applications"
11：10－11：50	Jan Musfeldt *(University of Tennessee, USA)* "Dynamical Charge and Structural Strain in MoS2 and MnO Nanoparticles"
11：50－12：30	Sheng Dai *(Oak Ridge National Laboratory, USA)* "Self-Assembly Synthesis and Functionalization of Nanoporous Carbon Materials for Energy-Related Applications"
12:30	Lunch (IOP Restaurant)
13：30－15：50	**Session 7** *Chair: Hong Guo*
13：30－14：00	Min Ouyang *(Maryland University, USA)* "Engineering Fundamental Spin and Charge Interactions at the Nanoscale"
14：00－14：40	Feng Liu *(University of Utah, USA)* "Collective Magnetic Behavior of Graphene Nanohole Superlattices"
14：40－15：20	Xiaoqing Yang *(Brookhaven National Lab, USA)* "Structural Changes of Nano-sized LiFePO4-LiMnPO4 Solid Solutions Studied by In-situ XRD"

15：20－15：50	Yongsheng Hu *(Institute of Physics, CAS, China)* “Nanostructured Molybdenum Oxides as Anode Materials for Lithium-Ion Batteries”
15：50－16：00	Coffee Break
16：00－18：20	**Session 8** *Chair: Andreas J. Heinrich*
16：00－16：40	Greber Thomas *(Physics Institute, University of Zurich, Switzerland)* “Functional Nano-templates: sp2 Single Layer Superstructures”
16：40－17：20	Xudong Xiao *(Chinese University of Hongkong)* “Smallest Electric Rectifier by Selective Wave Function Coupling”
17：20－18：00	Tiehan Shen *(University of Salford, UK)* “The Measurement of Stokes Parameters and Its Application to the Study of Magneto Optical Properties of Nanostructured Materials”
18：00－18：20	Qing Huan *(PhD student, IOP, CAS)* “Spatial Images of Different Vibornic Peaks at Single Molecule Level”

July 3　IOP Building D 212	
	Session 9 *Chair: Jian Shen*
8：30－9：00	Chonglin Chen *(University of Texas, San Antonio, USA)* "Interface Engineered Nanostructural Metamaterials with Anomalous Physical Phenomena"
9：00－9：40	Yi Shi *(Nanjing University, China)* "Selective Epitaxial Semiconductor Nanowires and their Applications"
9：40－10：10	Zhaohua Cheng *(Institute of Physics, CAS, China)* "Manipulation of Magnetic Anisotropy and Domain Structure of Co Nanodots on Pb/Si Substrates by Step Decoration"
10：10－10：40	Qingsong Huang *(Institute of Physics, CAS, China)* "Formation of Centimeter–scale Epitaxial Graphene on 4H-SiC by Pulsed Electron Irradiation"
10：40－11：00	Haitao Yang *(Institute of Physics, CAS, China)* "Achieving a Noninteracting Magnetic Nanoparticle System through Direct Control of Interparticle Spacing"
11：00－11：20	Yi Pan *(PhD student, IOP, CAS)* "Fabrication and Application of High Quality Graphene Monolayer on Ru (0001)"
Closing Remarks	

Quantum Magnetism of Atoms on Surfaces: An STM Study

Andreas J. Heinrich

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Understanding and controlling the magnetic properties of nanoscale systems is crucial for the implementation of future data storage and computation paradigms. Magnetic data storage is currently limited by the amount of magnetic anisotropy per atom and computation by the large amount of energy dissipation. Hence studies at the ultimate limit of miniaturization are of paramount importance for future IT applications.
Here we show how the magnetic properties of individual atoms and artificially created nanostructures can be probed with a low-temperature, high-field scanning tunneling microscope when the atoms are placed on a thin insulator (see Fig. 1). We find clear evidence of very large magnetic anisotropy in the spin excitation spectra of individual magnetic atoms embedded in this surface [1]. The STM allows the determination of all parameters in the corresponding Spin Hamiltonian which describes the quantized energy levels of the spin system in real-space and under application of external magnetic fields.
In extended one-dimensional spin chains (see Fig. 2), which we build one atom at a time on the surface, we find strong spin-coupling into collective quantum-spins, even for the longest chains of length 3.5nm [2]. The spectroscopic results can be understood with the model of spin-excitations in a system with antiferromagnetic Heisenberg coupling, controlled on the atomic scale.
We will discuss recent advances in spin excitation spectroscopy through the application of spin-polarized tunneling currents [3]. At low current densities, the well-characterized spectra of Mn and Fe on Cu2N allow a quantitative determination of the degree of spin-polarization. At high current densities, the spin-polarized current can exert a significant torque on the magnetic atoms and nanostructures, culminating in the steady-state occupation of highly excited spin-states. In analogy to the classical spin-transfer torque, the direction of the tunneling current determines the occupation of the spin states of the quantum spin systems.

1. C.F. Hirjibehedin, C-Y Lin, A.F. Otte, M. Ternes, B.A. Jones, C.P. Lutz, and A.J. Heinrich, *Science* **317**, 1199 (2007).
2. C.F. Hirjibehedin, C.P. Lutz, A.J. Heinrich, *Science* **312**, 1021 (2006).
3. S. Loth, K. von Bergmann, M. Ternes, C. P. Lutz, and A. J. Heinrich, *to be published*.

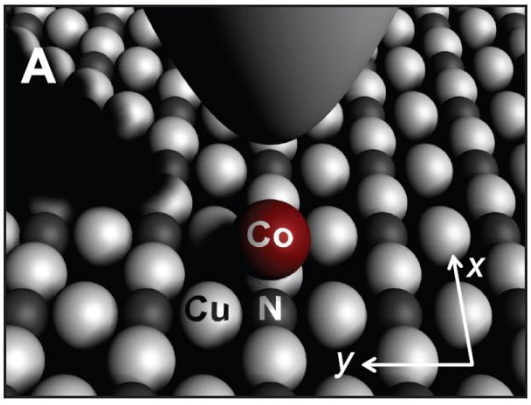

FIG. 1. Magnetic atoms are placed on top of a thin insulating layer and probed with STM.

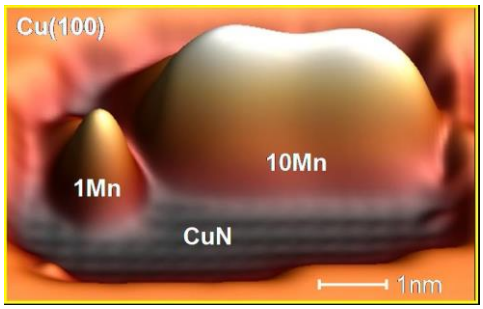

Fig. 2. Topographic image of a single Mn atom on Cu2N next to a chain of 10 Mn atoms which was assembled with the STM.

Dynamic Processes Observed by Scanning Tunnelling Microscopes: Conformation Changes, Diffusion and Vibrations

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Since its invention scanning tunnelling microscopes have rapidly become the key instrument not only for the atomic scale analysis of surfaces, interfaces, and molecular structures, the instrument's resolution has made it increasingly possible to detect electronic processes which before remained elusive. Driven by experimental advances sophisticated theoretical techniques have been developed, which make direct comparisons with quantitative results a close to routine procedure. The key ingredient in these techniques is the inclusion of the STM tip in the simulations, and the use of highly accurate electronic structure methods. In this talk we shall focus on dynamic processes, which increasingly play an important role in state-of-the-art experiments. We shall limit our presentation to two fields of research: magnetic nanostructures and molecular corrals. In particular we show that the field-induced diffusion of adsorbates to the probe tip can change the magnetic resolution in the experiments by nearly one order of magnitude [1], and that the tip field will change the Kondo temperature of a single magnetic impurity in a continuous manner during its approach [2,3]. In case of single Ce adatoms on silver we find that a Kondo-like feature, which is only observed under particular experimental conditions, is due to hydrogen diffusion and subsequent vibrational excitations [4]. This is also important in the context of a previously reported Kondo effect for the Ce/Ag system [5], which in light of the theoretical analysis and new experimental evidence has to be subject to revision. Our second focus, molecular corrals on silicon surfaces, starts with an analysis of semiconductor properties upon adsorption of highly polar chlorododecane molecules [6,7]. Here, we show that the induced surface dipole due to the polar charge distribution changes the bandstructure of the semiconductor within the molecular corral to an extent usually observed only after semiconductor doping. Most interestingly, this effect is revealed as a consequence of only minor changes of the molecular conformation [8,9]. This research seems to open up the possibility of tailoring local semiconductor properties by molecular adsorption.

[1] WA Hofer et al. *Phys. Rev. Lett.* **100**, 026806 (2008)
[2] L. Limot et al. *Phys. Rev. Lett.* **94**, 126102 (2005)
[3] N. Neel et al. *Phys. Rev. Lett.* **98**, 016801 (2007)
[4] WA Hofer et al., *Nanotechnology* **19**, 305701 (2008)
[5] J. Li et al., *Phys. Rev. Lett.* **80**, 2893 (1998)
[6] S. Dobrin et al., *Nanotechnology* **18**, 044012 (2007)
[7] S. Dobrin et al., *Surf. Sci. Lett.* **600**, L43 (2006)
[8] KR Harikumar et al., *JACS* **128**, 16791 (2006)
[9] KR Harikumar et al., Nature Nanotechnology **3**, 222 (2008)

Characterization of Point Defects on MgO(001) Films

Jichun Lian[1], Thomas Risse[2], Hajo Freund[2], Hongjun Gao[1]

1. Institute of Physics, Chinese Academy of Sciences, Beijing, China
2. Fritz -Haber-Insitut der MPG, Department of Chemical Physics, Berlin, Germany

Surface point defects, including adatoms, clusters, and vacancies, plays a very important role in a variety of technologically fields such as heterogeneous catalysis. In this respect it is particularly important to understand the role of defect sites and their interaction with gas molecules, which may alter the surface properties significantly. In our group, we have investigated several systems such as Ge adatoms on Si(111)-7×7 surface[1] , defect structure of the CeO_2(111) films[2] and Li atoms on MgO(001) surface[3]. In the present study, we use a combination of infrared (IR) and electron paramagnetic resonance (EPR) spectroscopy to characterize the electronic properties of copper atoms and clusters and their interaction with surface color centers on MgO(001) films. By adsorbing CO molecules, a Cu-di-carbonyl like species as well as the mono carbonyl was found. The formation of these carbonyl species can be understood by the presence of single Cu atoms at low temperature. EPR spectra are capable to prove the nucleation of copper on the paramagnetic color centers. Consistently, the intensity of the IR signals of CO on color centers decreased or vanished after copper deposition.

[1]Y.L.Wang, H.-J.Gao, H.M.Guo,*et.al.* **Phys. Rev. Lett.** 94,106101(2005)
[2]J.-L.Lu, H.-J.Gao, S.Shaikhutdinov, H.-J. Freund, **Sur. Sci.** 600,5004(2006)
[3]J.C.Lian, T.Risse, H.-J.Gao, H.-J.Freund,*et.al.* **Chem. Phys. Lett.** 450,308(2008)

Symmetry Mismatch and Reversible Polymorphism in Two Dimensional Molecular Crystals

Leo Merz,[a] Manfred Parschau,[a] Tobias Bauert,a Jay S. Siegelb & Karl-Heinz Ernst[a,b]

a) Molecular Surfaces Science, Empa – Swiss Federal Laboratories for Materials Testing and Research, Dübendorf, Switzerland
b) Organic Chemistry Institute, University of Zürich, Switzerland

Crystallization of organic compounds is one of the most important means in chemical and pharmaceutical industry to obtain products. But many chemical compounds exist in more than one crystalline form, and these so called polymorphs often show very different physical properties. Control of polymorphism is therefore of vital importance in food processing, pharmaceuticals, speciality chemicals and even optical data storage. Although solid-solid phase transitions have been scientifically studied for almost 200 years, they are still poorly understood. A promising approach is to study these two-dimensional (2D) crystallization phenomena on well-defined substrates with scanning tunneling microscopy (STM) and other surface sensitive techniques. Understanding self-assembly phenomena of organic molecules at metal surfaces is also important for new materials systems for photovoltaic and organic electronics. We investigate symmetry mismatch effects in crystallization, by 2D tiling with fivefold-symmetric corannulene derivatives, so-called buckybowls. STM reveals interesting strategies to achieve close-packing where the symmetry actually does not allow perfect tiling. Entropic contributions from excited vibrations in 2D corannulene lattices on Cu(111) stabilize certain polymorphs at higher temperatures. Changing the temperature then interconverts reversibly the polymorph via so-called enantiotropic phase transitions. The detailed study of the microscopic mechanism of these phase transitions via STM allows to interfere with these processes and to select a polymorph by phase transition blocking due to lateral confinement of the molecules.

Direct Probe of the Key Building Block of the Fe-based Superconductors with Scanning Tunneling Microscopy/Spectroscopy (STM/S)

Shuheng H. Pan

Department of Physics/Texas Center for Superconductivity, University of Houston

The recently discovered superconductivity in iron (Fe)-based compounds is another exciting advancement in condensed matter physics since the discovery of high-Tc superconductivity in cuprates. Using a UHV Low Temperature Scanning Tunneling Microscope, we have been studying the structural and electronic properties of the parent and Co-doped BaFe2As2 compound. We find that, by low temperature in situ cleaving, we are able to expose the key building block – the Fe-As layer of this compound, where superconductivity is believed to occur. With STM/S, we directly probe this key building block with spatial resolution down to atomic scale. STM is a surface sensitive technique. Keeping this in mind, I will demonstrate how we use this high real-space resolution and surface sensitive technique to learn the structural and electronic properties within the bulk. I will also discuss our results on the density-of-states (DOS) evolution with doping, the scaling of the superconducting energy gap, and some electronic local effects that may be used to help determine the pairing symmetry.

Atomic Simulation of Disorder Effects in Magnetic Tunnel Junctions

Hong Guo

Mcgill University, Canada

I will report a recent theoretical development for treating atomistic disorder in nonlinear and non-equilibrium quantum transport modeling. The theory uses non-equilibrium vertex corrections to handle the configurational average of random disorder at the density matrix level. Using this technique, we have analyzed spin injection in magnetic tunnel junctions with interface roughness and with oxygen vacancies in the tunnel barrier. Disorder effect is found to very significantly alter spin polarized tunneling.

Dephasing and Disorder Effects in Quantum Spin Hall Effect

X.C. Xie

Oklahoma State University and Institute of Physics, Chinese Academy of Sciences

The influence of dephasing on the quantum spin Hall effect (QSHE) is studied. In the absence of dephasing, the longitudinal resistance in a QSHE system exhibits the quantum plateaus. We find that these quantum plateaus are robust against the normal dephasing but fragile with the spin dephasing. Thus, these quantum plateaus only survive in mesoscopic samples. Moreover, the longitudinal resistance increases linearly with the sample length but is insensitive to the sample width. These characters are in excellent agreement with the recent experimental results [Science 318, 766 (2007)]. In addition, we define a new spin Hall resistance that also exhibits quantum plateaus. In particular, these plateaus are robust against any type of dephasing and therefore, survive in macroscopic samples and better reflect the topological nature of QSHE.

In addition, we also study the disorder effect on the transport properties in QSHE. We confirm that at a moderate disorder strength, the initially un-quantized two terminal conductance becomes quantized, and the system makes a transition to the novel topological Anderson insulator (TAI). Conductances calculated for the stripe and cylinder samples reveal the topological feature of TAI and supports the idea that the helical edge states may cause the anomalous quantized plateaus. The influence of disorder is studied by calculating the distributions of local currents. Base on the above-mentioned picture, the phenomena induced by disorder in the quantum spin Hall region and TAI region are directly explained.

Interference Phenomena in Superconducting Nb Thin Films Perforated with Periodic Hole Array

X.G. Qiu

National Laboratory for Superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

Artificial structure of hole arrays with a length scale of several tens nm have been fabricated on Nb thin films with electron beam lithography and reactive ion milling. Magnetic field dependent resistance has been measured at different temperatures near the superconducting transition temperature. Resistance minima have been observed when there are integer and fractal numbers of vortices at each hole. An explanation based on the interference between Cooper pairs is provided.

This work is incorporation with M. Kamran, A. D. Thakur, H. Cai, S. Ooi, K. Hirata, X. Hu, Y.G. Yao, T. Xiang, H.F. Yang, W.H. Cao, S.P. Zhao, Q. Niu, X.C. Xie.

Fig.1 1MJ/25KV pulsed power supply

Fig.2 Pulsed magnet

Fig.3 Two experiment stations

Spin Physics and Kondo Effect in Semiconductor Quantum Dots

Hongqi Xu

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I will report our recent study of spin physics and Kondo phenomena in semiconductor quantum dots. The devices were fabricated from semiconductor heterostructures and from semiconductor nanowires. Spin states, effective g-factors, spin-orbit interaction energy, and exchange energy were measured for the fabricated quantum dots. We also studied strong correlation phenomena and observed both odd-number electron and even-number electron Kondo effects in our fabricated quantum dot devices.

Theory of Directed Nucleation of Strained Islands on Patterned Substrates

Hao Hu[1,2,] Hongjun Gao[1], Feng Liu[2]

[1]*Nanoscal Physics and Devices Laboratory, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2]*Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112, USA*

To obtain quantum dots with highest spatial and size uniformity, people have focused efforts on directing island nucleation using lithographically patterned substrates recently. This approach appears intuitively obvious, but the underlying physical mechanisms can be rather complicated and remain poorly understood. We develop a theoretical model to elucidate the nucleation of strained islands on patterned substrates. We show that island nucleation is directed to the preferred sites by a much lower energy barrier and smaller critical size. Strain relaxation directs island nucleation to the bottom of a pit rather than the top of a ridge as commonly perceived, while large surface energy anisotropy is responsible for nucleation at both places. The theory explains some puzzling experimental results and provides useful guidelines for future exploration of directing the self-assembly of quantum dots on patterned substrates.

[1]B. Yang, F. Liu, M.G. Lagally, Phys. Rev. Lett. **92**, 025502 (2004)

[2]Hao Hu, Hongjun Gao, Feng Liu, Phys. Rev. Lett. **101**, 216102 (2008)

Emergent Phenomena in Spatially Confined Manganites

Jian Shen

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Colossal electroresistance, colossal magnetoresistance, high T_c superconductivity and the metal-insulator transition are some of the fascinating emergent behaviors found in complex materials; however there is as yet no known model that is capable of fully explaining any one of these behaviors let alone a unifying understanding capable of explaining the effects of complexity on emergent behavior as a whole. One common trait that many of these complex materials share is electronic phase separation. For this reason, a fuller understanding of electronic phase separation should have far reaching implications across a wide range of materials.

We will discuss recent work on a novel spatial confinement technique that has led to some fascinating new discoveries on the role of electronic phase separation (EPS) in manganites. In transport measurements on unconfined systems where device size is larger than the inherent electronic phase domains, current bypasses regions of high resistance in favor of regions with lower resistance, because the probing electrons will follow the path of least resistance. By confining complex materials exhibiting EPS to length scales smaller than the electronic phase domains that reside within them, it is possible to simultaneously probe multiple resistive regions. This method allows for a much more complete view of the phases residing in a material and gives vital information on phase formation, movement and fluctuation. Since these phase separated regions also posses varied properties, this technique promises to lead to unexpected functionalities for future device applications.

Reduced dimensionality studies on complex oxides sit at the intersection of fundamental science and technological application. With the wide range of useful materials—ferromagnets, antiferromagnets, high T_C superconductors, multiferroics—present in the complex oxides class, the burgeoning field of oxide electronics presents itself as the future of device design. Not only will spatial confinement studies on correlated systems give us new insights into fundamental physics, these studies are a vital step in the creation and implementation of practical oxide electronic devices. Further, the formation and coexistence of multiple electronic phases in a single system have been suggested as purely emergent phenomena[4]; establishing a common language capable of discussing complexity in these material systems could find overlap with other fields, such as Biology or Economics, where complex systems are the norm.

Gate-All-Around Silicon Nanowire Transistors from Top-Down Approach: Fabrication and Experimental Characterization

Ru Huang*, Runsheng Wang, Yu Tian, Liangliang Zhang, Jing Zhuge, Changze Liu, Yujie Ai, Yiqun Wang and Yangyuan Wang

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Due to the superior electrostatics, improved transport property and CMOS compatibility, gate-all-around silicon nanowire transistor (SNWT) attracted more attentions and shows great potentials for the ultimately-scaled devices. This paper mainly discusses a new process integration scheme based on bulk substrate, which features epi-free integration, self-aligned structure and large source/drain fan-out. The characteristics of the fabricated device with 10nm diameter nanowire were investigated. The transport behavior of the SNWTs is experimentally evaluated. A modified experimental extraction methodology of transport property for SNWTs is proposed, which takes into account the impact of temperature dependence of parasitic resistance. The sub-40nm SNWTs exhibit high ballistic efficiency at room temperature. Self-heating effect is also experimentally characterized and due to the 1-D nature of nanowire and increased phonon-boundary scattering in GAA structure, the self-heating effect in SNWTs based on bulk substrate is comparable or even a little bit worse than SOI devices, which may limit the ultimate performance of SNWT-based circuits. Special design consideration for SNWTs is expected.

This work is supported by National Natural Science Foundation of China (No. 60625403, 90207004), Special Funds for Major State Basic Research (973) Projects of China (2006CB302701).

Carbon Nanotubes and Graphene Nanoribbons

Hongjie Dai

Stanford University, USA

This talk will present our latest results on using carbon nanotubes for biological applications including SERS Raman tags for highly sensitive protein detection, multiplexed multicolor Raman imaging of cells and biological tissues, and near-IR imaging of biological systems. I will then switch to graphene nanoribbon work, including several methods we developed recently to form ribbons with narrow widths and smooth edges. Unzipping nanotubes to form graphene ribbons will be shown. Graphene edge chemical reactivity and a method of edge chemical functionalization will also be presented.

Post CMOS Nanoelectronics Research for the Next Generation Logic Switches

Chunyung Sung

T. J. Watson Research Center, IBM

CMOS scaling becomes extremely difficult beyond 15nm node because of limits to performance improvement and increasing power density from scaling . While multi-core technologies and other innovations will enable the industry to continue functional scaling for another 10-15 years, ultimately a new computing paradigm which is capable of representing, manipulating, and transmitting logic information with functional, power, and density advantages over CMOS needs to be found.

Towards Carbon Based Electronics

Philip Kim, Siu-Wai Chan
Columbia University, USA

This talk covers some of the latest advances on Graphene research at Columbia University

Functional Nanoparticles: Synthesis and Potential Applications

Shouheng Sun

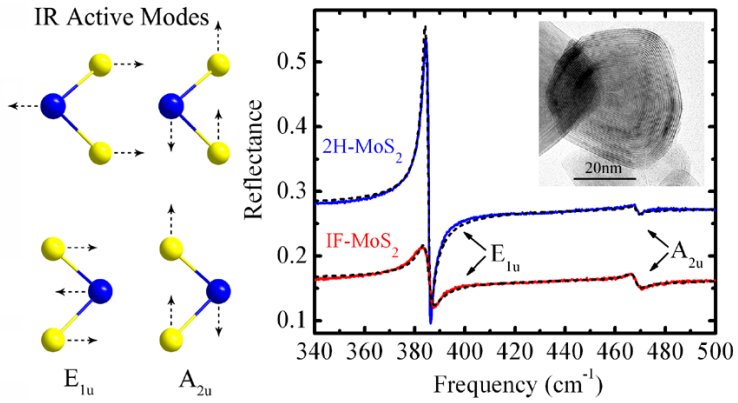
Department of Chemistry, Brown University, Providence, RI 02912, USA.

The talk focuses on the synthesis and applications of composite nanoparticles containing noble metal and iron oxide. Using solution phase based reduction chemistry, we have synthesized a series of monodisperse oleylamine-coated nanoparticles of Au and Pt. These noble nanoparticles could serve as seeds for the production of composite dumbbell-like NM-Fe3O4 (NM = Au, Pt) nanoparticles. Once functionalized with a special antibody, peptide and an antitumor agent, these nanoparticles can be made target-specific and are promising for medical diagnostics and therapeutics. In contrast, upon the removal of the surfactant, the Pt- or Au-based nanoparticles become highly active catalysts for oxygen reduction and CO oxidation.

Dynamical Charge and Structural Strain in MoS2 and MnO Nanoparticles

J.L. Musfeldt, Q.-C. Sun, X.S. Xu (University of Tennessee), A. Zak (NanoMaterials), R. Tenne (Weizmann), S. Baker and A. Christianson (ORNL)

In order to investigate finite length scale effects and chemical bonding in prototypical nanomaterials, we measured the far infrared vibrational properties of nanoscale MoS_2 and MnO. From an analysis of frequencies, oscillator strengths, and high-frequency dielectric constants, we extract Born and local effective charges for both materials and compare the results to their traditional bulk analogs. In MoS_2, we find that the intralayer Born effective charge of the nanoparticles is decreased significantly compared to the layered bulk, a difference that we attribute to the structural strain (and resulting change in polarizability) in the nanoparticles. In the MnO system, the Born effective charge of the nanoparticles is also decreased compared to the bulk material, although here, the local charge is also decreased, implying that confinement modifies ionicity. Thus, the nanoscale analogs of MoS_2 and MnO exemplify finite size effects on electronic polarizability and chemical bonding, respectively.



Mode	Material	Z_B^*(e)	α (Å^3)	Z^*(e)
E_{1u}	2H-MoS_2	1.11	100	0.15
	IF-MoS_2	0.69	91	0.16
A_{2u}	2H-MoS_2	0.52	200	0.37
	IF-MoS_2	0.52	200	0.37

Self-Assembly Synthesis and Functionalization of Nanoporous Carbon Materials for Energy-Related Applications

Sheng Dai

Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6201

Porous carbon materials are ubiquitous in separation, catalysis, and energy storage/conversion. Well-defined mesoporous carbon materials are essential for a number of the aforementioned applications. Ordered porous carbon materials have previously been synthesized using colloidal crystals and presynthesized mesoporous silicas as hard templates. The mesostructures of these carbon materials are connected via ultrathin carbon filaments and can readily collapse under high-temperature conditions. Furthermore, these hard-template methodologies are extremely difficult to adapt to the fabrication of large-scale ordered nanoporous films or monoliths with controlled pore orientations. More recently, my research group at the Oak Ridge National Laboratory and several others around the world have developed alternative methods for synthesis of highly ordered mesoporous carbons via self-assembly. Unlike the mesoporous carbons synthesized via hard-template methods, these mesoporous carbons are highly stable and can be graphitized at high temperature (>2800^{o}C) without significant loss of mesopores. The surface properties of these materials can be further tailored via surface functionalization. This seminar will provide an overview and perspective of the mesoporous carbon materials derived from soft-template synthesis and surface functionalization and their fascinating applications in catalysis, separation, and energy storage devices.

Engineering Fundamental Spin and Charge Interactions at the Nanoscale

Min Ouyang

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Metal and semiconductor nanostructures show many unusual properties and functionalities, and can serve as model system to explore fundamental quantum and classical coupling interactions as well as building blocks of many practical applications. In this talk I will focus on some of our recent work in controlling fundamental spin and charge interactions by tuning fine structures at the nanoscale. I will start by presenting how to apply chemical synthetic strategy to tune nanocrystallinity and core-shell structures with precision nano-tailoring. Enabled by such, fundamental properties including electron-phonon, phonon-phonon, and plasmonic interactions can be dramatically modified. Other than chemical strategy, I will also highlight that both structure and spin interactions within semiconductor quantum dots can be manipulated by for example high pressure technique. These discussions should offer important implications for our understanding of the fundamental properties at nanoscale and potential applications of nanostructures.

Collective Magnetic Behavior of Graphene Nanohole Superlattices

Feng Liu

University of Utah, USA

We predict a new class of 2-D crystalline “bulk” magnets—the graphene nanohole (GNH) superlattices with each GNH acting like a “super” magnetic atom, using first principles calculations. We show that such superlattices can exhibit long-range magnetic order above room temperature, with a collective magnetic behavior governed by inter-NH spin spin interactions in additional to intra-NH spin ordering. Furthermore, magnetic semiconductors can be made by doping magnetic NHs into semiconducting NH superlattices. The possibility of engineering magnetic GNHs for storage media and spintronics applications is discussed.

Structural Changes of Nano-sized $LiFePO_4$-$LiMnPO_4$ Solid Solutions Studied by In-situ XRD

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Since the pioneer work of Goodenough's research group, olivine-structured $LiMPO_4$ (M= Fe, Mn, Co and Ni) compounds have been studied intensively as cathode materials for lithium ion batteries due to its good safety characteristics and high thermal and chemical stabilities. The lithiation and delithiation process of $LiFePO_4$ can be explained by a two-phase mechanism of through the coexistence of $LiFePO_4$ and $FePO_4$ phases. In order to increase the energy density, other transition metal substituted iron phosphates have been synthesized and studied. The $LiMn_yFe_{1-y}PO_4$ system is one of them. In this system, the structural changes are more complicated than the un-substituted $LiFePO_4$ and many of the details are not fully understood yet. In addition, the electrochemistry performance of $LiFe_{1-y}Mn_yPO_4$ solid solution has a strong relationship to the content of Mn, as well as the particle size of the materials. In order to further understand the mechanism of electrochemical lithition and delithiation process of $LiFePO_4$-$LiMnPO_4$ solid-solution, we have synthesized a series of $Li_xFe_{1-y}Mn_yPO_4$ samples with different "y" value with nano-size particles and performed in-situ XRD experiments during charge and discharge processes. It was found that the structural changes of these materials depend on many factors, such as the Mn content, the charge-discharge rates, as well as the electrochemical history of the samples. The details of these results will be reported in the meeting.

Acknowledgement

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Nanostructured Molybdenum Oxides as Anode Materials for Lithium-Ion Batteries

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Nanostructured materials have attracted great interest in the field of lithium-ion batteries essentially because of their substantial advantages concerning mass transport. Transport in nanoparticle systems typically encompasses shorter transport lengths for both electronic and Li^+ transport, higher electrode/electrolyte contact area, better accommodation of the strain of Li insertion/extraction and in some cases also local anomalies.

In this presentation, various nanostructured molybdenum oxides such as mesoporous MoO_2, MoO_2 nanorods, MoO_3 nanobelts have been investigated for Li storage.[1-3] Compared with micrometer-sized MoO_2, nanostructured MoO_2 shows significantly improved Li storage performance in terms of reversible capacity and cycling performance. A surprising finding is that the reversible capacity gradually increases upon cycling for the nanostructured MoO_2 electrode. The reason still remains unknown. Extensive characterizations show that Li-storage mechanism in MoO_2 may be not a conversion reaction as some other transition metal oxides e.g. Fe_3O_4, Co_3O_4 do. In contrast to MoO_2 and reference 4, the electrochemical Li storage behavior of MoO_3 abides by a conversion reaction mechanism, i.e. $MoO_3 + 6Li \rightarrow Mo + 3Li_2O$. A stable reversible capacity of 750 mA h g^{-1} was obtained for MoO_3 nanobelts whereas the capacity decayed rapidly for micrometer-sized MoO_3. Present studies provide further examples of advantages of nanostructured materials in the field of lithium-ion batteries.

Acknowledgements

The authors are indebted to Chinese Academy of Sciences and acknowledge support in the framework of the 100 Talent Project. The authors would like to thank the following collaborators: Prof. Liquan Chen, Dr. B. Guo, Prof. G. D. Stucky, Dr. Y. Shi, Dr. R. Seshadri.

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Functional Nano-templates: sp2 Single Layer Superstructures

Greber Thomas

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A functional nano-template enables self-assembly of otherwise impossible arrangements of molecules. This has e.g. been observed at room temperature for the case of naphthalocyanine, a molecule with 2 nm diameter, on hexagonal boron nitride nanomesh h- BN/Rh(111) [1]. Here the template function is related to lateral electric fields (dipole rings) on the nanometer scale [2]. For the case of smaller molecules like water two separated phases within the superstructure unit cell were observed [3]. Like hexagonal boron nitride, graphene also forms mismatch driven single layer superstructures on transition metals. If these two sp2 hybridized layer systems are compared, it is found that their template function is related to dipole rings, though with different signs and strength, where the metallicity of graphene allows better screening of the lateral electrostatic fields [4]. From this a three level hierarchy model for sp2 templates is proposed, where the sp2 sigma bonds provide the robustness of the layers, the pi bonds the adsorption energies and the weakest the “alpha” bonds the lateral trapping.\

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Smallest Electric Rectifier by Selective Wave Function Coupling

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Hong Kong, China

Electric rectification is a basic function in modern microelectronics and in future nanoelectronics. We found that a cluster consisting of as few as three Ag atoms or three Au atoms deposited on Si(111)-(7×7) surface can behave as a strong electric rectifier, with a rectification ratio as large as ~150, when measured with the surface as one electrode and an STM tip as another. Based on first-principles calculations, we analyzed the spatial extension of the wave functions of the Ag cluster in the surface normal direction and found that the wave functions for quantum states at different energies spill out of the surface to different extent. Such wave function distribution provides an opportunity for selective energy states coupling. We demonstrated by theoretical simulations and experimental coupling changes that the observed rectification is a result of coupling the STM tip with wave functions of selective energy states of the clusters, different from the Schottky effect and the effect of the total density of electronic states.

The Measurement of Stokes Parameters and Its Application to The Study of Magneto Optical Properties of Nanostructured Materials

Tiehan H. Shen

Joule Physics Laboratory, Institute for Materials Research, University of Salford, U.K.

We derive a generalized methodology of photoelastic modulator based system designed for the measurement of the Stokes parameters of an arbitrary light beam. Based on the methodology, a critique of various potential configurations that could be used to effect such measurements is presented. Calibration procedures for the entire optical system is introduced which, among other things, renders a knowledge of the frequency response of the detector system unnecessary. An analysis of the errors due to incorrect setting of optical components is presented for some of the more practical cases. This allows an assessment of the relative merit of different experimental configurations.

Nanocomposite films consisting of regularly ordered iron nanowires embedded in anodic aluminium oxide templates have been fabricated and their magneto-optical properties studied by determining the four Stokes parameters of the transmitted laser beam originally linearly polarized and at normal incidence to the film surfaces. The results of the nanowire arrays are found to be considerably different from that of bulk iron. While an increase in diameter of the nanowire leads to a substantial increase in the values of the Faraday rotation angles per unit length at a fixed value of the magnetic fields, they are substantially less than that of bulk iron, indicating that the effective media theory may not be directly applicable. The magneto optical characteristics of other magnetic nanowire arrays will also be presented.

Spatial Images of Different Vibornic Peaks at Single Molecule Level

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Spatial distributions of different vibronic peaks on single naphthalocyanine molecules adsorbed on an ultrathin aluminum oxide film are imaged by a scanning tunneling microscope in real space at low temperature. The spatial variations of electron-vibronic coupling in these images reveal the interplay between the molecular comformation, the vibrational modes and the molecular orbital structure, which are in accordance with spectra recorded at different locations over the molecule. This work shows that vibronic imaging can provide rich information of electron-vibrational coupling at the single molecule level.

Interface Engineered Nanostructural Metamaterials with Anomalous Physical Phenomena

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Interface engineered materials have attracted more and more attention in the multifunctional materials research and active device fabrication. It plays a key role to control the physical properties of advanced nanomaterials and results in the discovery of various new physical phenomena with excellent opportunity for developing new metamaterials for active devices and engineered nanosystems. We have focused on the systematical studies on the formations and the characterizations of various highly epitaxial oxide thin films and multilayered layered structures to understand the nature of interface induced anomalous physical phenomena. Recently, we have achieved an excellent dielectric tunability of 80% from highly epitaxial ferroelectric Mn:(Ba,Sr)TiO_3 thin films from the interface controlled nano domain structures and observed strong anisotropic phenomena in highly epitaxial (Pb,Sr)TiO_3 thin films; setup a new record of giant magnetoresistance ratio of 10^{10} (four order higher than the previous record) from the artificial interface domain structured (La,Ca)MnO_3 epitaxial thin films; and observed an anomalous clamped domain ferroelectric phenomena from the multilayered $BaTiO_3$/$SrTiO_3$ superlattices. A series of models were developed to understand these interface phenomena.

Selective Epitaxial Semiconductor Nanowires and their Applications

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The ability to rationally synthesize semiconductor nanowires (NWs) with precisely controlled and tunable chemical composition, size, structure and morphology and to accurately dope them with both *p*- and *n*- type dopants has opened up opportunities for bottom-up assembling almost any kind of functional nanosystem ranging from electronics to optoelectronics and photonics. Impressive progress in this field has been made in the last few years. In this talk, we will discuss selective epitaxial NWs used for electrically driven lighting devices.

Nanoscale patterned template offers a good platform for selective epitaxial growth over a wide range of compound semiconductor materials. The advantage of this method is the easy integration of the NWs into devices, and the good electrical contact between NWs and substrate. InGaN NWs have been fabricated on SiO_2 by MOCVD templates. The primary results have indicated that the present method can be used for the fabrication of the NWs with various densities and symmetries for a wide range of semiconductor materials.

Manipulation of Magnetic Anisotropy and Domain Structure of Co Nanodots on Pb/Si Substrates by Step Decoration

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Co nanodots are fabricated by means of molecular beam epitaxial (MBE) on the Pb/Si substrates with 0.1° miscut and 4° miscut along (111) direction, respectively. Scanning tunneling microscope (STM) images indicated that Co nanodots distribute randomly on the wide terrace of 0.1° miscut Pb/Si(111) substrate, while quasi-one-dimensional Co chains are formed along the step edge direction of the 4° miscut Pb/Si substrate. Both *in situ* surface magneto-optical Kerr effect (SMOKE) and magnetic force microscopy (MFM) measurements demonstrate that step decoration can induce a transformation of uniaxial magnetic anisotropy and Neel domain walls for quasi-one-dimensional Co chains from isotropic and cross-tie like domain walls for randomly distributed Co nanodots. Furthermore, quantitative analysis indicates the effective magnetic anisotropy constant of quasi-one-dimensional Co chains is about $4.1\times10^{4}\mathrm{J/m^{3}}$ in terms of domain wall width. This step decoration provides an additional means to manipulate magnetic anisotropy of surface-supported magnetic nanodots.

Formation of centimeter-scale epitaxial graphene on 4H-SiC by pulsed electron irradiation

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The new discovery of graphene, a single basal layer of graphite as a strict two-dimensional material, could be classified into two types: freestanding graphene, usually suspended on SiO_2/Si substrate by "peeling off" or chemical process, and epitaxial graphene (EG) mainly grown on SiC or metals. So far, since EG grown carefully on SiC is electronically the same as an ideally isolated graphene sheet and even has more intriguing properties (*eg*. Opening a bandgap in electronic spectra of EG), and considering the epitaxial graphene on SiC is most likely to harness in future applications for the post-Moore's law electronics and highly sensitive electro-mechanical devices.More and more attentions have focused on preparing EG by graphitization of hexagonal SiC surface with heat annealing (TA). However, large-scale production of graphene with high quality and tunable number of layers on SiC substrate could not yet be realized by now. Here we show a novel route to graphene on SiC substrate based on Pulsed Electron Deposition system (PED). This new route allows us to obtain graphene in a large area up to Centimeter-Sized by the irradiation of electrons with tunable incident energy and position. Meanwhile the number of layers is 1 to 3 in most of so-formed graphene. As a host material for next generation semiconductor, the large epitaxial graphene sheets have opened a door for us to explore future graphene-based devices.

Formation of centimeter-scale epitaxial graphene on 4H-SiC by pulsed electron irradiation

Achieving a Noninteracting Magnetic Nanoparticle System through Direct Control of Interparticle Spacing

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Magnetic nanoparticles (NPs) represent a critical link between current technology and the next generation of magnetic materials, because of their intriguing physical properties including superparamagnetic behavior and spin glass behavior. These unique properties are often ascribed to the delicate interplay between intrinsic properties and magnetostatic interactions. Dispersion of NPs in insert media such as SiO_2, Al_2O_3, a polymer matrix, and a liquid suspension to form a granular film or a magnetic fluid is currently being used to study the dipolar interactions of magnetic NPs. However, it is very difficult to avoid aggregation completely in order to obtain isolated particles and to control the interparticle spacing, since some magnetic clusters exist even in extremely dilute solutions. In addition, this method cannot provide data for very high particle concentrations due to agglomeration. So there has been a great challenge: controlling the interparticle spacing, and thus dipolar interaction, for each particle even in a dense particle system. The direct manipulation of the interparticle spacing for each particle, would promote the experimental investigation of interparticle interaction based on some theoretical predictions.

Since magnetite (Fe_3O_4) has a higher saturation magnetization (M_s, 89 emu/g) than magnetite (Fe_2O_3, 79 emu/g) and better chemical stability than iron, Fe_3O_4 particles are a good candidate for studying magnetostatic interactions. In this paper, monodisperse superparamagnetic Fe_3O_4 NPs were synthesized and coated using a nonmagnetic SiO_2 shell with controlled thickness ranging from 3.0 to 20.0 nm. The temperature-dependent zero-field-cooled (ZFC) and field-cooled (FC) magnetization of the resultant 7.5 nm Fe_3O_4 nanoparticles with systematically increasing interparticle spacing were studied using the continuous and intermittent cooling protocol. The experimental evidence and simulated ZFC/FC curves using actual parameters from TEM images reveal that the increasing interparticle spacing modulated the collective magnetic behavior by effectively lowering the interparticle dipolar coupling, and for 7.5 nm Fe_3O_4 nanoparticles a noninteracting particle system formed with interparticle spacing above 31.5 nm.

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Fabrication and Application of High Quality Graphene Monolayer on Ru (0001)

Yi Pan, Min Gao, Li Huang, Haigang Zhang, Jinhai Mao, Hongjun Gao
Institute of Physics, Chinese Academy of Sciences, Beijing 100090, P. R. China

we report a method for fabrication large scale single layer graphene by thermal annealing of ruthenium single crystal containing carbon. Low energy electron diffraction (LEED) indicates the graphene grows to as large as millimeter dimensions with good long-range order, and scanning tunneling microscope (STM) shows continuity and perfect crystallinity. Analysis of Moiré pattern augmented with first-principles calculations shows the graphene layer is incommensurate with the underlying Ru(0001) surface forming superlattice with an average lattice strain of ~ +0.81%. Our findings offer an effective method for producing high quality single crystalline graphene for fundamental research and further application.

“中科院-国家外专局纳米材料与器件研究国际合作团队”
（四川大学部分）
International Workshop on Nanomaterials and Nanodevices

(Sichuan University, July 6-7, 2009)

地点（Venue)：Sichuan University

Scientific Program	
Welcome Remarks: Jie GAO (Sichuan University) Hong GUO (Mcgill University/Sichuan University)	
8：30 -10：30	**Session1** *Chair: Min Gong*
8：30 - 9：10	Jie Gao *(Sichuan University, China)* “Single Electrons Transport Induced by the Surface Acoustic Waves in Semiconductor Heterostructures”
9：10－9：50	Hongjie Dai *(Stanford University, USA)* “Carbon Nanotubes and Graphene Nanoribbons”
9：50－10：30	Tiehan Shen *(University of Salford, UK)* “The Measurement of Stokes Parameters and Its Application to the Study of Magneto Optical Properties of Nanostructured Materials”
	Coffee Break and Photos
10：40－12：00	**Session 2** Chair: Chunyung Sung?
10：40－11：20	Chunyung Sung *(T. J. Watson Research Center, IBM)* “Post CMOS Nanoelectronics Research for the Next Generation Logic Switches “
11：20－12：00	Andreas J. Heinrich (Almaden Research Center, IBM) “Measuring the Force to Move an Atom on a Surface”
12：00	Lunch （Sichuan University Restaurant)
13：30－15：30	**Session 3** Chair: Jian Shen
13：30－14：10	Shuheng Pan *(University of Houston, USA)* “Direct Probe of the Key Building Block of the Fe-based Superconductors with Scanning Tunneling Microscopy/Spectroscopy (STM/S)”
14：10－14：50	Sheng Dai *(Oak Ridge National Laboratory, USA)* “Self-Assembly Synthesis and Functionalization of Nanoporous Carbon Materials for Energy-Related Applications”

14：50－15：30	Siu-Wai Chan *(Columbia University,USA)* "Synthesis and Redox Behavior of Copper Oxide and Manganese Oxide Nanoparticles"
15：30－15：40	Coffee Break
15：40－18：00	**Session 4** Chair: Siu-Wai Chan
15：40－16：20	Jan Musfeldt *(University of Tennessee, USA)* "Finite Size Effects and Solid State Lubrication in Nanoscale WS2"
16：20－17：00	Hong Guo *(Mcgill University, Canada)* "Au/BDT Molecular Transport Junction: Can DFT get it right？"
17：00－17：40	Thomas Greber *(Physics Institute, University of Zurich, Switzerland)* "Substrates for Molecular Spintronics "
17：40－18：20	Hongjun Gao *(Institute of Physics, CAS, China)* "A Site-specific Kondo Effect at Ambient Temperatures in Iron-based Molecules and the Modulation"
18：20	Dinner MIN GONG (Director of the Physics College, SU): Welcoming Speech

8：30－10：30	**July 7th, 2009** **Session 5** Chair: Thomas Greber
8：30－9：10	Ke Xia *(Beijing Normal University,China)* "First-principles Study of Spin-transfer Torques in Layered Systems with Textured Magnetization"
9：10－9：50	Qingfeng Sun *(Institute of Physics, CAS, China)* "Controllable Andreev Retroreflection and Specular Andreev Reflection in a Four-terminal Graphene-superconductor Hybrid System"
9：50－10：30	Yuan Lin *(University of Electronic Science and Technology of China)* "Use of Strain to Tune the Physical Properties of Nanoscale Ferroelectric Thin Films"
	Coffee Break and Photos (photo-taking is repeated and should be cancelled)
10：40－12：00	**Session 6** Chair:Hong Guo
10：40－11：20	Chonglin Chen *(University of Texas, San Antonio, USA)* "Interface Engineered metamaterials with optimized ionic transport ptoperties for Solid State Fuel Cells"
11：20－12：00	Peng Li *(Sichuan University,China)* "Bond-operator Mean-field Theory of a Generalized Frustrated SU(N) Model and Its Applications To the Spin Lattice Models"
12：00－12：30	Lixiang Cen *(Sichuan University,China)* " First-Order Quantum Phase Transitions in Matrix Product Systems: Latent Observable and Multipartite Entanglement Scaling"
12：30	Closing Remarks Hongjun Gao (Institute of Physics, CAS, China) Jian Shen (Oak Ridge National Laboratory, USA)

Single Electrons Transport Induced by the Surface Acoustic Waves in Semiconductor Heterostructures

Jie Gao
Sichuan University, China

Carbon Nanotubes and Graphene Nanoribbons

Hongjie Dai
Stanford University, USA

This talk will present our latest results on using carbon nanotubes for biological applications including SERS Raman tags for highly sensitive protein detection, multiplexed multicolor Raman imaging of cells and biological tissues, and near-IR imaging of biological systems. I will then switch to graphene nanoribbon work, including several methods we developed recently to form ribbons with narrow widths and smooth edges. Unzipping nanotubes to form graphene ribbons will be shown. Graphene edge chemical reactivity and a method of edge chemical functionalization will also be presented.

The Measurement of Stokes Parameters and Its Application to The Study of Magneto Optical Properties of Nanostructured Materials

Tiehan H. Shen

Joule Physics Laboratory, Institute for Materials Research, University of Salford, U.K.

We derive a generalized methodology of photoelastic modulator based system designed for the measurement of the Stokes parameters of an arbitrary light beam. Based on the methodology, a critique of various potential configurations that could be used to effect such measurements is presented. Calibration procedures for the entire optical system is introduced which, among other things, renders a knowledge of the frequency response of the detector system unnecessary. An analysis of the errors due to incorrect setting of optical components is presented for some of the more practical cases. This allows an assessment of the relative merit of different experimental configurations.

Nanocomposite films consisting of regularly ordered iron nanowires embedded in anodic aluminium oxide templates have been fabricated and their magneto-optical properties studied by determining the four Stokes parameters of the transmitted laser beam originally linearly polarized and at normal incidence to the film surfaces. The results of the nanowire arrays are found to be considerably different from that of bulk iron. While an increase in diameter of the nanowire leads to a substantial increase in the values of the Faraday rotation angles per unit length at a fixed value of the magnetic fields, they are substantially less than that of bulk iron, indicating that the effective media theory may not be directly applicable. The magneto optical characteristics of other magnetic nanowire arrays will also be presented.

Post CMOS Nanoelectronics Research for the Next Generation Logic Switches

Chunyung Sung

T. J. Watson Research Center, IBM

CMOS scaling becomes extremely difficult beyond 15nm node because of limits to performance improvement and increasing power density from scaling . While multi-core technologies and other innovations will enable the industry to continue functional scaling for another 10-15 years, ultimately a new computing paradigm which is capable of representing, manipulating, and transmitting logic information with functional, power, and density advantages over CMOS needs to be found.

Quantum Magnetism of Atoms on Surfaces: An STM Study

Andreas J. Heinrich

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Understanding and controlling the magnetic properties of nanoscale systems is crucial for the implementation of future data storage and computation paradigms. Magnetic data storage is currently limited by the amount of magnetic anisotropy per atom and computation by the large amount of energy dissipation. Hence studies at the ultimate limit of miniaturization are of paramount importance for future IT applications.
Here we show how the magnetic properties of individual atoms and artificially created nanostructures can be probed with a low-temperature, high-field scanning tunneling microscope when the atoms are placed on a thin insulator (see Fig. 1). We find clear evidence of very large magnetic anisotropy in the spin excitation spectra of individual magnetic atoms embedded in this surface [1]. The STM allows the determination of all parameters in the corresponding Spin Hamiltonian which describes the quantized energy levels of the spin system in real-space and under application of external magnetic fields.
In extended one-dimensional spin chains (see Fig. 2), which we build one atom at a time on the surface, we find strong spin-coupling into collective quantum-spins, even for the longest chains of length 3.5nm [2]. The spectroscopic results can be understood with the model of spin-excitations in a system with antiferromagnetic Heisenberg coupling, controlled on the atomic scale.
We will discuss recent advances in spin excitation spectroscopy through the application of spin-polarized tunneling currents [3]. At low current densities, the well-characterized spectra of Mn and Fe on Cu2N allow a quantitative determination of the degree of spin-polarization. At high current densities, the spin-polarized current can exert a significant torque on the magnetic atoms and nanostructures, culminating in the steady-state occupation of highly excited spin-states. In analogy to the classical spin-transfer torque, the direction of the tunneling current determines the occupation of the spin states of the quantum spin systems.

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2. C.F. Hirjibehedin, C.P. Lutz, A.J. Heinrich, *Science* **312**, 1021 (2006).
3. S. Loth, K. von Bergmann, M. Ternes, C. P. Lutz, and A. J. Heinrich, *to be published*.

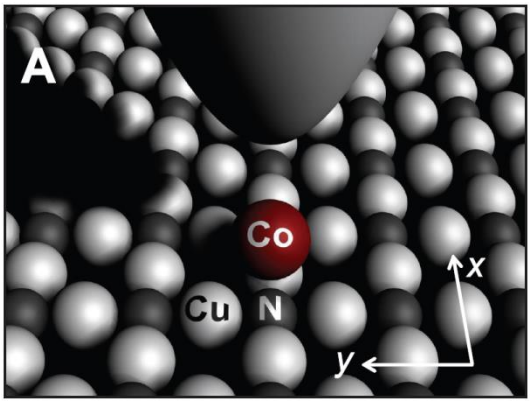

FIG. 1. Magnetic atoms are placed on top of a thin insulating layer and probed with STM.

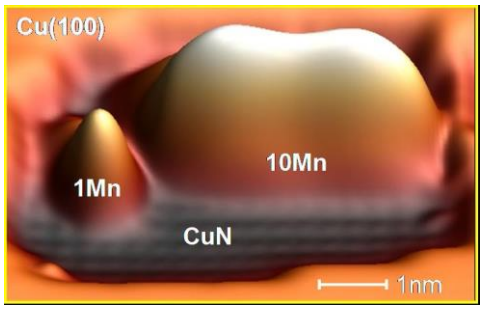

Fig. 2. Topographic image of a single Mn atom on Cu2N next to a chain of 10 Mn atoms which was assembled with the STM.

Self-Assembly Synthesis and Functionalization of Nanoporous Carbon Materials for Energy-Related Applications

Sheng Dai

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Porous carbon materials are ubiquitous in separation, catalysis, and energy storage/conversion. Well-defined mesoporous carbon materials are essential for a number of the aforementioned applications. Ordered porous carbon materials have previously been synthesized using colloidal crystals and presynthesized mesoporous silicas as hard templates. The mesostructures of these carbon materials are connected via ultrathin carbon filaments and can readily collapse under high-temperature conditions. Furthermore, these hard-template methodologies are extremely difficult to adapt to the fabrication of large-scale ordered nanoporous films or monoliths with controlled pore orientations. More recently, my research group at the Oak Ridge National Laboratory and several others around the world have developed alternative methods for synthesis of highly ordered mesoporous carbons via self-assembly. Unlike the mesoporous carbons synthesized via hard-template methods, these mesoporous carbons are highly stable and can be graphitized at high temperature (>2800^{o}C) without significant loss of mesopores. The surface properties of these materials can be further tailored via surface functionalization. This seminar will provide an overview and perspective of the mesoporous carbon materials derived from soft-template synthesis and surface functionalization and their fascinating applications in catalysis, separation, and energy storage devices.

Synthesis and Redox Behavior of Copper Oxide and Manganese Oxide Nanoparticles

Siu-Wai Chan
Columbia University, USA

Finite Size Effects and Solid State Lubrication in Nanoscale WS2

J.L. Musfeldt, Sonal Brown, Q.C. Sun, R. Luttrell (University of Tennessee), I. Mihut, J.B. Betts, A. Migliori (Los Alamos), A. Zak (NanoMaterials), R. Tenne (Weizmann)

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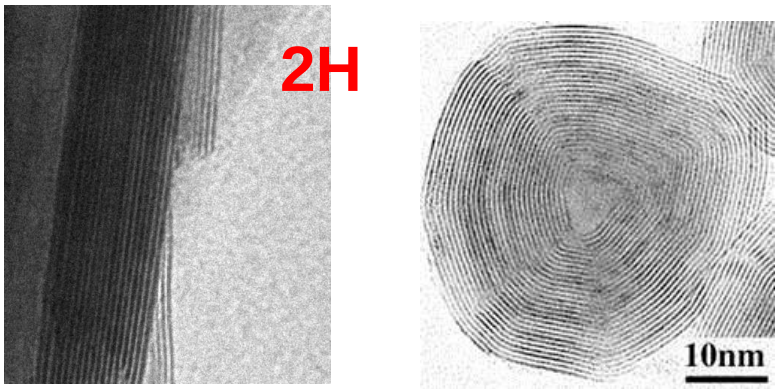
Understanding complexity at the nanoscale is one of the ``grand challenges" in the physical sciences. With their unprecedented functionality, opportunity for novel chemistry, and exciting new foundational physics, nanomaterials are emerging as a class of compounds with enormous transformational potential. In this talk, I will focus on the issue of phonon confinement, discussing our recent measurements of acoustic phonons in model materials. Specific systems of interest include transition metal dichalcogenides (such as 2H- and IF-WS2) and complex oxides such as the spinels. In each case, we work with both traditional bulk analogs + chemically identical but morphologically different nanoscale materials. These measurements reveal extraordinary phonon confinement effects, the mechanisms of which I will discuss in terms of local bonding, finite length scale effects, and strain-induced changes in local chemistry. I will also discuss the impact of finite length scale effects on the engineering properties of WS2.



Au/BDT Molecular Transport Junction: Can DFT get it right

Hong Guo

Mcgill University, Canada

Substrates for Molecular Spintronics

Thomas Greber

Physics Institute, University of Zurich, Switzerland

The control of the spin degree of freedom in molecules -a prerequisite for molecular spintronics - is obtained with various approaches. Here the ferromagnetic surface the Ni(111) that is expected to transfer magnetization to adsorbates is described. In order to characterize the spin dynamics at the surface, spin polarized photoemission and X-ray circular dichroism are applied.

A Site-specific Kondo Effect at Ambient Temperatures in Iron-based Molecules and the Modulation

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Due to their importance in the emerging field of molecular electronics, the transport properties of single molecules have been the focus of intensive research. Magnetic properties of transition metal atoms in a host molecule can be detected by a Kondo resonance in cryogenic scanning tunneling microscopes. These properties are important variables in the fabrication of single molecule devices. In this talk, I will present measurements of the Kondo effect of iron phthalocyanine (FePc) molecules on an Au(111) surface. Our results indicate a high Kondo temperature, well above room temperature, for the FePc molecule adsorbed on Au(111) surface. It is further revealed that a substantial change of the effect is with the adsorption configuration of the molecule. Furthermore, magnetic properties of an interface can be controlled at the molecular level by site-specific adsorption and modification of molecular structures. We verify by first-principles calculations that the molecular environment alters the hybridization of spin-polarized states of the molecule with states of the metal substrate, and that this alteration depends on the adsorption site of the molecule. The finding opens up the possibility to tailor magnetic properties of an organic interface to the desired specifications.

Collaborators: L. Gao,[1] Q. Liu,[1] Y.Y. Zhang,[1] N. Jiang,[1] H.G. Zhang,[1] S.X. Du,[1] and W.A. Hofer[2]. [1]*Institute of Physics, Chinese Academy of Sciences, China;* [2]*University of Liverpool, UK*

First-principles Study of Spin-transfer Torques in Layered Systems with Textured Magnetization

Ke Xia

Beijing Normal University

The electric current passing through a conducting (anti)ferromagnet is polarized, leading to spin-transfer torques when the order parameter is textured, such as in (anti)ferromagnetic noncollinear spin valves and domain walls. An efficient first-principles method was developed to calculate spin-transfer torques with noncollinear magnetization. The complete scattering wave function is determined by matching the wave function in the scattering region with the Bloch states in the leads. The spin-transfer torques are obtained with the aid of the scattering wave function. We applied our method to the magnetic domian walls and found that the material Co, Ni, and Ni_80Fe_20 dependence of the spin-transfer torques could be well understood by the Fermi surfaces. Ni has much longer spin injection penetration length than Co.

Controllable Andreev Retroreflection and Specular Andreev Reflection in a Four-terminal Graphene-superconductor Hybrid System

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We report the investigation of electron transport through a four-terminal graphene-superconductor hybrid system. The Andreev reflection coefficients and the conductance are obtained using non-equilibrium Green function method. Due to the quantum interference of the reflected holes from two graphene-superconductor interfaces with phase difference θ, it is found that the specular Andreev reflection vanishes at $\theta=0$ while the Andreev retroreflection disappears at $\theta=\pi$. This means that the retroreflection and specular reflection can be easily controlled and separated in this device. In addition, the reflected hole exhibits wave or particle behavior depending on the device's size. For small sample size, the wave behavior is dominant. Therefore the reflected hole can exit from both graphene terminals. For large sample size, however, the particle behavior manifests. Then the reflected hole only exit from a particular graphene terminal depending on the type of Andreev reflection.

Use of Strain to Tune the Physical Properties of Nanoscale Ferroelectric Thin Films

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Perovskite ferroelectric materials have been considered as a kind of extraordinary important functional materials due to their attractive physical properties. However, it has been found that the properties of these thin films are quite different from those of their bulks. Especially, when the thickness of the films scaled down to nanometers, the interfacial strain is believed to play a significant role in the properties of the thin films. In this presentation, we use (Pb,Sr)TiO3 (PSTO) thin films as an example to discuss how to use the strain to tune the physical properties of nanoscale ferroelectric thin films. The PSTO films were epitaxially grown on various single crystal substrates. Microstructures of the films were investigated using high resolution x-ray diffraction and electron microscopy while the dielectric properties were characterized. Crystal distortion and interface relationships were compared. PSTO films on LaAlO3 and MgO exhibit a tetragonal distortion whereas the film on NdGaO3 substrate shows an orthorhombic distortion. The orientation of the film is related to the fabrication condition such as cooling rate. Strain relaxation during the growth of the films was discussed. Dielectric properties of the films show a strong correlation with the strain.

Interface Engineered metamaterials with optimized ionic transport ptoperties for Solid State Fuel Cells

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The last few decades have seen an explosion in the development of new materials chemistry for sustainable energy devices, driven in parallel by the demands of technology and the inquisitiveness of basic sciences and engineering. In particular, Solid State Fuel Cells (SOFCs) have promised a high-energy efficiency and can provide society with sustainable energy producing technology. In the past ten years, we have systematically studied various highly mixed conductive and ionic conductive materials and focused on the acquisition of fundamental understanding the physical properties and chemical stability of advanced nanostructured materials when used in multilayered structures for the development of an intermediate temperature solid oxide fuel cell (IT-SOFC). Our efforts have demonstrated that the highly ionic conductive $PrBaCo_2O_5$ is a good cathode candidate for IT- SOFC. The interface engineered YSZ/GCO multilayered structures can significantly enhance the oxygen exchange in the electrolyte. Also, various interesting transport properties have been observed in the mixed conductive $LaBaCo_2O_{5.5}$. Details will be discussed in the talk.

Bond-operator Mean-field Theory of a Generalized Frustrated SU(N) Model and Its Applications to the Spin Lattice Models

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A class of symmetrically frustrated SU(N) model is constructed. The general model reduces to the familiar XXZ model, spin-1 bilinear-biquadratic model, and the spin-orbital model for N=2,3,4 respectively. The formalism facilitates the introduction of boson or fermion representation and the corresponding mean-field theory based on the bond-operator decomposition. As an application of the theory, its solution of the well-known Haldane chain is presented. Its application to the two-dimensional spin liquid system is also addressed.

First-Order Quantum Phase Transitions in Matrix Product Systems: Latent Observable and Multipartite Entanglement Scaling

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Despite that first-order classical phase transitions are hackneyed in thermal equilibrium systems, the species of counterparts of quantum phase transitions (QPTs) are less understood and few results for them are available. Here, through a renewed composite regime, we report paradigms of first-order QPTs and fundamental physics in models of matrix product systems. The quantum ground state under construction is shown to exhibit abrupt transitions in the first derivative of Z, a partition function over local bases. In analogy with classical liquid-gas phase transitions, these QPTs are signaled by emergence of a physical quantity so called as latent observable whose expectation value detects precisely the jump of the derivative of the logarithm of Z. Furthermore, our studies on scaling properties for the established system reveal that the global multipartite entanglement plays an essential role in dominating the behavior of the first-order QPTs.