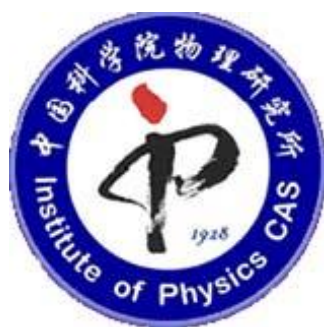


**2012 International Workshop on  
Nanomaterials & Nanodevices**

**July 9<sup>th</sup>-16<sup>th</sup>, Beijing-Xining, China**



**July 9<sup>th</sup>-11<sup>th</sup>, 2012**

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

**July 12<sup>th</sup>-16<sup>th</sup>, 2012**

**Qinghai University, Xining, China**

Institute of Physics, Chinese Academy of Sciences  
Bureau of Science and Technology, Qinghai Province  
Qinghai University

**中国科学院物理研究所纳米材料与器件国际研讨会  
(北京部分)**

**International Workshop on Nanomaterials and Nanodevices**

(Beijing Part, July 9<sup>th</sup>-11<sup>th</sup>, 2012)

**Scientific Program**

<b>July 9<sup>th</sup>, Monday, IOP Building D 212</b>	
8: 30—8: 40	<b>Opening Ceremony and Welcome Remarks</b> <b>Hongjun Gao</b> ( <i>Institute of Physics, CAS, China</i> )
8: 40—10: 40	<b>Session 1</b> <i>Chair: W. A. Hofer</i>
8: 40—9: 20	<b>Andreas J. Heinrich</b> ( <i>Almaden Research Center, IBM, USA</i> ) “The Quantum and Classical Properties of Spins on Surfaces”
9: 20—9: 50	<b>Xincheng Xie</b> ( <i>Peking University, China/Oklahoma State University, USA</i> ) “The Topological System with a Twisting Edge Band”
9: 50—10: 20	<b>Thomas Greber</b> ( <i>University of Zurich, Switzerland</i> ) “sp <sup>2</sup> Hybridized Single Layer Honeycomb Templates”
10: 20—10: 40	Photo and Coffee Break

10: 40—12: 00	<b>Session 2</b> <i>Chair: Andreas J. Heinrich</i>
10: 40—11: 20	<b>Chih-Kang Shih</b> ( <i>University of Texas at Austin, USA</i> ) “Quantum Control of Boundary Conditions in Ultra-thin Superconducting Films”
11: 20—12: 00	<b>W. A. Hofer</b> ( <i>The University of Liverpool, UK</i> ) “Dynamic Processes Observed by Scanning Tunneling Microscopes: Vibrations, Diffusions and Reactions”
12: 00	Lunch ( IOP Restaurant )

<b>Session 3</b>	
<i>Chair: Harald Fuchs</i>	
13: 30–14: 10	<b>Hongjie Dai</b> ( <i>Stanford University, USA</i> ) “Novel Materials for Nanoscience and Nanotechnology”
14: 10–14: 50	<b>Shengbai Zhang</b> ( <i>Rensselaer Polytechnic Institute, USA</i> ) “Excited-State Dynamics: An <i>Ab Initio</i> Study of Photoinduced Hydrogen Desorption from Hydrogenated Graphene”
14: 50–15: 20	<b>Xuan Gao</b> ( <i>Case Western Reserve University, USA</i> ) “One-dimensional Quantum Confinement Effect Modulated Thermoelectric Properties in InAs Nanowires”
15: 20–15: 50	<b>Dapeng Yu</b> ( <i>Peking University, China</i> ) “Electrical-Mechanical Coupling in Bent ZnO Nano/Microwires”
15: 50–16: 00	Coffee Break

<b>Session 4</b>	
<i>Chair: Peter Varga</i>	
16: 00–16: 30	<b>Jiandi Zhang</b> ( <i>Louisiana State University, USA</i> ) “Why are Ultrathin Films of Metallic Oxides not Metallic”
16: 30–17: 00	<b>Feng Liu</b> ( <i>Utha University, USA</i> ) “A Combination of Strain Induced Nanoscale Self-Assembly and Strain Engineered Band Structure”
17: 00–17: 30	<b>Chonglin Chen</b> ( <i>University of Texas at San Antonio, USA</i> ) “Multiphase, Multistructure, and Multifunctionality in Interface Engineered Thin Films”
17: 30–18: 00	<b>Sheng Meng</b> ( <i>Institute of Physics, CAS, China</i> ) “Interface Energy Conversion at the Nanoscale: Insights from Ultrafast Electron Dynamics”

<b>July 10<sup>th</sup>, Tuesday, IOP Building D 212</b>	
8: 30–10: 20	<b>Session 5</b> <i>Chair: Hongjie Dai</i>
8: 30–9: 10	<b>Hans-Joachim Freund</b> ( <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i> ) “Ultrathin Oxide Films: the “Physics” of Catalysis”
9: 10–9: 40	<b>Zhong Fang</b> ( <i>Institute of Physics, CAS, China</i> ) “Topological Insulators and Topological Semimetals”
9: 40–10: 10	<b>Hong-Jun Gao</b> ( <i>Institute of Physics, CAS, China</i> ) “Growth and Si-Layer Intercalation of Centimeter-scale, Highly-ordered, Continuous Graphene on Metal Surfaces for Future Integrated Electronic Devices”
10: 10–10: 20	Coffee Break

10: 20–11: 50	<b>Session 6</b> <i>Chair: Thomas Greber</i>
10: 20–11: 00	<b>Harald Fuchs</b> ( <i>University of Münster, Germany</i> ) “Chemistry on Nanostructured Templates”
11: 00–11: 30	<b>Jenny-Zhen Yu</b> ( <i>RF Nano Corporation, USA</i> ) “Nanoelectronics Based on Carbon Nanotubes”
11: 30–11: 50	<b>Haitao Zhou</b> ( <i>Institute of Physics, CAS, China</i> ) “STM Investigation of Organic Molecules on Graphene/Ru(0001) ”
11: 50	Lunch ( IOP Restaurant )

<b>Session 7</b>	
<i>Chair: Hans-Joachim Freund</i>	
13: 30–15: 40	
13: 30–14: 10	<b>Peter Varga</b> ( <i>Vienna University of Technology, Austria</i> ) “Oxides as Templates for Metal Nano-Cluster”
14: 10–14: 40	<b>Guanyu Zhang</b> ( <i>Institute of Physics, CAS, China</i> ) “Direct Growth of Graphene and its Applications in Sensors and Memories”
14: 40–15: 10	<b>Ming Liu</b> ( <i>Institute of microelectronics, CAS, China</i> ) “Rectifying-Based RRAM Crossbar Array for High Density Storage Applications”
15: 10–15: 30	<b>Wuxia Li</b> ( <i>Institute of Physics, CAS, China</i> ) “Freestanding Nanostructures for Three-Dimensional Nanodevices”
15: 30–15: 40	Coffee Break

<b>Session 8</b>	
<i>Chair: Chonglin Chen</i>	
15: 40–17: 40	
15: 40–16: 10	<b>Zhaohua Cheng</b> ( <i>Institute of Physics, CAS, China</i> ) “Controllable Magnetic Anisotropies of Epitaxial Fe/Si(111) Films Manipulated by Current treating”
16: 10–16: 40	<b>Bingbing Liu</b> ( <i>Jilin University, China</i> ) “High Pressure Induced Novel Phase Transition in Nanostructured Materials”
16: 40–17: 10	<b>Zhenchao Dong</b> ( <i>University of Science and Technology of China, China</i> ) “Exploring Single-Molecule Electroluminescence through Nanocavity Plasmons”
17: 10–17: 40	<b>Hong Li</b> ( <i>Institute of Physics, CAS, China</i> ) “Structure Evolution of Li <sub>2</sub> MnO <sub>3</sub> for Li-ion Batteries”

<b>July 11<sup>th</sup>, Wednesday, IOP Building D 210</b>	
8: 30—11: 00	<b>Session 9</b> <i>Chair: Shengbai Zhang</i>
8: 30—9: 00	<b>Anping Li</b> ( <i>Oak Ridge National Laboratory, USA</i> ) “Electron Transport at the Nanoscale”
9: 00—9: 30	<b>Leonid Lichtenstein</b> ( <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i> ) “The Atomic Arrangement in Two-Dimensional Silica – From Crystalline to Vitreous Structures”
9: 30—10: 00	<b>Jing Tao</b> ( <i>Brookhaven National Laboratory, USA</i> ) “Probing Nanoscale Phase Separation in Colossal Magnetoresistive Manganites”
10: 00—10: 30	<b>Yeliang Wang</b> ( <i>Institute of Physics, CAS, China</i> ) “Understanding Multiple Interactions in Functional Nanostructures of QA Molecules at Metal Surfaces”
10: 30—10: 50	<b>Liwei Liu</b> ( <i>Institute of Physics, CAS, China</i> ) “Molecule-substrate Coupling between Metal Phthalocyanines and Epitaxial Graphene Grown on Ru(0001) and Pt(111)”
10: 50—11: 00	<i>Closing Remarks: Hongjie Dai</i>

**中国科学院物理研究所纳米材料与器件国际研讨会  
(西宁部分)**

**International Workshop on Nanomaterials and Nanodevices**

(Xining Part, July 12<sup>th</sup>, 2012)

**Scientific Program**

8: 30— 9: 00	<b>Opening Ceremony and Welcome Remarks</b>
8: 30—8: 45	<b>Shuguang Bian</b> ( <i>Bureau of Science and Technology of Qinghai Province</i> ) Welcome Remarks
8: 45—9: 00	<b>Xidong Liang</b> ( <i>Qinghai University, China</i> ) Introduction to Qinghai University
9: 00—10: 40	<b>Session 1</b> <i>Chair: Hongjie Dai</i>
9: 00—9: 30	<b>Hans-Joachim Freund</b> ( <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i> ) “Nanoparticles as Models for Heterogeneous Catalysts: An Atomic View”
9: 30—10: 00	<b>Feng Liu</b> ( <i>Utha university, USA</i> ) “A Combination of Strain Induced Nanoscale Self-Assembly and Strain Engineered Band Structure”
10: 00—10: 30	<b>Andreas J. Heinrich</b> ( <i>Almaden Research Center, IBM, USA</i> ) “The Quantum and Classical Properties of Spins on Surfaces”
10: 30—10: 40	Coffee Break

10: 40—12: 00	<b>Session 2</b> <i>Chair: Andreas J. Heinrich</i>
10: 40—11: 10	<b>W. A. Hofer</b> ( <i>The University of Liverpool, UK</i> ) “TiO <sub>2</sub> : Fundamentals, Applications, and Perspectives”
11: 10—11: 40	<b>Shengbai Zhang</b> ( <i>Rensselaer Polytechnic Institute, USA</i> ) “Dirac Fermion in Strongly-Bounded Graphene Systems”
11: 40—12: 00	<b>Shixuan Du</b> ( <i>Institute of Physics, CAS, China</i> ) “Molecules on Moiré Template of Graphene Monolayer Grown on Ru(0001)”
12: 00	Lunch

13: 30–14: 40	<b>Session 3</b> <i>Chair: Harald Fuchs</i>
13: 30–14: 00	<b>Hongjie Dai</b> ( <i>Stanford University, USA</i> ) “Novel Materials for Nanoscience and Nanotechnology”
14: 00–14: 30	<b>Chonglin Chen</b> ( <i>University of Texas, San Antonio, USA</i> ) “Multiphase, Multistructure, and Multifunctionality in Interface Engineered Thin Films”
14: 30–14: 40	Coffee Break

14: 40–16: 20	<b>Session 4</b> <i>Chair: Feng Liu</i>
14: 40–15: 10	<b>Thomas Greber</b> ( <i>University of Zurich, Switzerland</i> ) “Spin Shuttles”
15: 10–15: 40	<b>Peter Varga</b> ( <i>Vienna University of Technology, Austria</i> ) “Oxides as Templates for Metal Nano-Cluster”
15: 40–16: 10	<b>Anping Li</b> ( <i>Oak Ridge National Laboratory, USA</i> ) “Electron Transport at the Nanoscale”
16: 10–16: 20	Coffee Break

16: 20–17: 40	<b>Session 5</b> <i>Chair: Hans-Joachim Freund</i>
16: 20–16: 50	<b>Harald Fuchs</b> ( <i>University of Münster, Germany</i> ) “Quantitative Surface Analysis and Generation of Complex Biomimetic Structures by AFM”
16: 50–17: 20	<b>Jing Tao</b> ( <i>Brookhaven National Laboratory</i> ) “Probing Nanoscale Phase Separation in Colossal Magnetoresistive Manganites”
17: 20–17: 40	<b>Wende Xiao</b> ( <i>Institute of Physics, CAS, China</i> ) “Graphene Epitaxy on Ru(0001): a Template for Supramolecular Nano-Architectures”
17: 40	<i>Closing Remarks: W. A. Hofer</i>



# Beijing Part

## **The Quantum and Classical Properties of Spins on Surfaces**

*Andreas J. Heinrich*

*Almaden Research Center, IBM, USA*

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The scanning tunneling microscope has been an extremely successful experimental tool because of its atomic-scale spatial resolution. In recent years this has been combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with microvolt energy resolution. In this talk I will review recent developments in investigating the electronic and magnetic properties of atoms and small clusters of atoms on surfaces. A particular focus will be on the use of magnetic materials for future device applications in the Information Technology industries.

A large enough cluster of magnetic atoms on a surface behaves similar to a macroscopic magnetic particle: its magnetization points along an easy-axis direction in space and magnetization reversal requires sufficient thermal energy to overcome a barrier. How many atoms does it take to create such a magnet? What are the size limits of stable magnetic nanoparticles. Those are important questions for our future technologies.

When the number of atoms in a cluster becomes small quantum tunneling of magnetization can take place and hence quantum mechanics can no longer be ignored but rather takes center stage. Single atoms that are slightly decoupled from conducting substrates behave more like quantum mechanical entities. These quantum systems can be studied with inelastic tunneling spectroscopy, a technique we coined spin-excitation spectroscopy. With this approach it is possible to measure the energy eigenstates of the quantum spin Hamiltonian that describes spins on surfaces with high precision.

## **The Topological System with a Twisting Edge Band**

*Xincheng Xie*

*Peking University, China*

*[xcxie@pku.edu.cn](mailto:xcxie@pku.edu.cn)*

We study a topological system with one twisting edge-state band and one normal edge-state band. For the twisting edge-state band, Fermi energy goes through the band three times, thus, having three edge states on one side of the sample; while the normal edge band contributes only one edge state on the other side of the sample. In such a system, we show that it consists of both topologically protected and unprotected edge states, and as a consequence, its Hall resistance depends on the location where the Hall measurement is done even for a translationally invariant system. This unique property is absent in a normal topological insulator.

## **sp<sup>2</sup> Hybridized Single Layer Honeycomb Templates**

*Thomas Greber*

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*greber@physik.uzh.ch*

Single layers of carbon or boron nitride may be easily grown on transition metals. A lattice mismatch between these sp<sup>2</sup> hybridized layers and the substrate imposes superstructures with a lattice constant in the nanometer range, where lateral electric fields are found to guide the assembly of molecules [1]. The structure of graphene on Ru(0001) will be discussed in view of tunneling microscopy, electron [2] and x-ray diffraction experiments [3]. Also, the stability of these nanostructures in air and liquids will be addressed in view of applications in future nano-devices.

[1] Surface Trapping of Atoms and Molecules with Dipole Rings Dil et al., *Science* **319** (2008) 1826.

[2] Structure Determination of the Coincidence Phase of Graphene on Ru(0001) Moritz et al., *Phys. Rev. Lett.* **104** (2010) 136102.

[3] Graphene on Ru(0001): A 25x25 Supercell Martoccia et al., *Phys. Rev. Lett.* **101** (2008) 126102.

## Quantum Control of Boundary Conditions in Ultra-thin Superconducting Films

*Chih-Kang Shih*

*Department of Physics, University of Texas at Austin, USA*

*[shih@physics.utexas.edu](mailto:shih@physics.utexas.edu)*

Studies of two-dimensional (2D) superconductivities have long been a topic of great fundamental interests. Recent advancements of materials synthesis have enabled the growth of epitaxial superconductor thin films with unprecedented control in crystallinity, atomic smoothness and film thickness, thus opening up new opportunities in investigations of 2D superconductivity. Indeed, studies of superconducting properties of ultra-thin Pb films on Si or Ge substrates have revealed several new aspects of 2D superconductivity, such as, quantum oscillations of the superconducting order parameter as a function of the film thickness. More significantly, even at a thickness of one or two atomic layers, the superconductivity remains relatively strong. It is noted that these ultra-thin film (from one to a few atomic layers) are grown on semiconductor substrates which provide a very effective isolation electronically. The intrinsically collective electronic phenomenon of superconductivity, on the other hand, is anticipated to be strongly influenced by its environment. More specifically when the superconductors are in contact with normal metals, induced superconductivity (proximity effect) is resulted. Here we present recent result in this regard. Two very different aspects of proximity effect are investigated.

The first aspect concerns lateral proximity effect in a 2D heterogeneous superconductor system comprised of 2D superconducting islands on top of a surface metal. By directly imaging how superconducting order propagates spatially we report intriguing influences of junction geometry on the proximity effect. Depending on the local geometry, the superconducting gap induced in the surface metal region can either be confined to the boundary of the superconductor, in which the gap decays within a short distance ( $\sim 20$  nm), or can be observed nearly uniformly up to several times of coherence lengths due to multiple Andreev reflections. In addition, the curvature at junction interface impacts the proximity length.

The second aspect concerns superconductivity of a bi-metallic heterojunction system formed with atomic precision. Molecular beam epitaxy is used to form superconductor - noble metal heterojunction whose interface is controlled with atomic abruptness. In addition, the thickness of each constituent of the bi-metallic system is controlled with atomic precision. It is found that the superconductivity of the composite is well accounted for by the Cooper model with thickness ranging from a few atomic layers to hundreds of monolayers. This is in stark contrast with earlier studies using granular films where significant deviations from Cooper model were found in the very thin regime. In addition to extracting model parameter which offers new insight into the pairing process in such composite structures, we found that an extension of the Cooper model also offer a novel resolution for recent controversies in thickness dependence of transition temperature of ultra-thin superconductors bounded by semiconductors.

## **Dynamic Processes Observed by Scanning Tunneling Microscopes: Vibrations, Diffusions and Reactions**

*W. A. Hofer*

*The University of Liverpool, UK*

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Dynamic processes in scanning tunneling microscopy (STM) are increasingly the focus of cutting edge research due to their importance for energy conversion and reaction processes. It is in principle possible to study these processes by suitable adaptation of STM theory and a step-by-step analysis of the processes themselves. I shall give several examples where such a detailed understanding is indispensable for a comprehensive understanding e.g. in atomic switching and diffusion processes, in molecular growth processes, condensation reactions, and long range molecular propagation even on reactive surfaces. At the end of my talk I shall demonstrate that careful statistical analysis in combination with high-resolution STM can even lead to surprising new insights into fundamental physics.

## **Novel Materials for Nanoscience and Nanotechnology**

*Hongjie Dai*

*Department of Chemistry, Stanford University, Stanford, California 94305, USA*

*[hdai1@stanford.edu](mailto:hdai1@stanford.edu)*

This talk will present our work on carbon nanotubes, graphene nanoribbons and graphene-inorganic hybrid nanomaterials. Biological applications of carbon nanotubes will be discussed including a new fluorescence imaging method in the so called NIR-II region in the spectral window of 1000-1400nm. NIR fluorescence enhancement of carbon nanotubes and organic fluorophores will be presented on a novel plasmonic substrate for 3D molecular tracking and biological detection. I will then talk about graphene nanoribbons, including several methods recently developed in our lab to form high quality graphene nanoribbons with narrow widths and smooth edges. Lastly, I will talk about our recent work on making inorganic nanoparticles and nanocrystals on graphene sheets for energy storage and electrocatalytic applications.

## **Excited-State Dynamics: An Ab Initio Study of Photoinduced Hydrogen Desorption from Hydrogenated Graphene**

*Shengbai Zhang*

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Understanding excited-state dynamics is critical for the study of light-matter interaction with important applications such as optoelectronics, photovoltaics, and photocatalysis. Photo-excitation can induce atomic desorption from a material in ways that are often counterintuitive and at variance with the predictions from ground-state dynamics. Taking hydrogenated graphene as an example, *ab initio* molecular dynamics, coupled with time-dependent density functional theory (TDDFT), reveals a hydrogen-coverage-dependent energy transfer process for photo-excited carriers with qualitatively different hydrogen ion dynamics. For example, sparsely populated H on graphene is difficult to dissociate, despite their thermodynamic instability. This inability can be attributed to the inefficient transfer of the excitation energy into the kinetic energy of the H under such a chemical environment. In contrast, H can be easily dissociated from fully hydrogenated graphene, despite its thermodynamic stability. One can trace this dynamic instability of hydrogen to the Coulomb repulsion between neighboring H ions, as a result of the charge transfer between graphene and hydrogen. Work is in collaboration with Junhyeok Bang and Fei Gao (PNNL).



## **One-dimensional Quantum Confinement Effect Modulated Thermoelectric Properties in InAs Nanowires**

*Xuan Gao*

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Thermoelectric properties have been measured in InAs nanowires synthesized by chemical vapor deposition (CVD) method. Gate modulation of the thermopower of individual InAs nanowires is obtained over the whole temperature range studied ( $T= 300\text{K}$  to  $40\text{K}$ ). At low temperatures ( $T < \text{c.a. } 100\text{K}$ ), large oscillations in the thermopower and power factor are observed to concomitant with the stepwise conductance increases as the gate voltage shifts the chemical potential of electrons in InAs nanowire through quasi-one-dimensional (1D) sub-bands. This work experimentally demonstrates the possibility to tailor materials' thermoelectric properties through 1D electronic confinement, a long sought-after goal in thermoelectrics research.

## Electrical-mechanical Coupling in Bent ZnO Nano/microwires

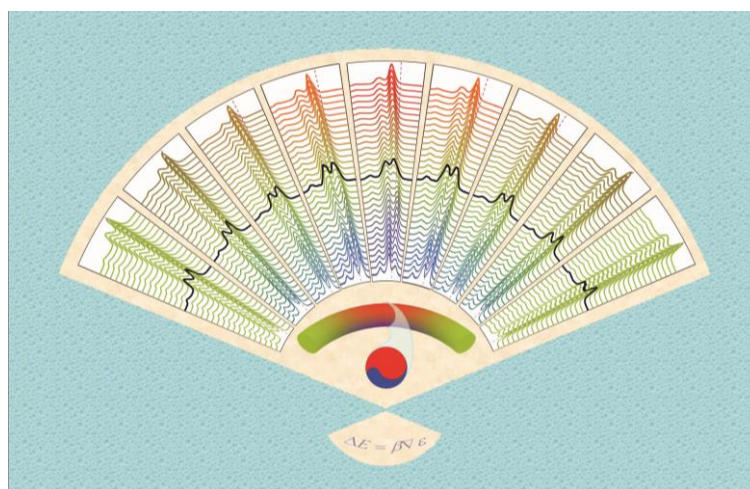
Xuewen Fu<sup>1</sup>, Xiaobing Han<sup>1</sup>, Ziyue Zhang<sup>2</sup>, Zhuhua Zhang<sup>2</sup>, Xinli Zhu<sup>1</sup>, Rui Zhu<sup>1</sup>, Jun Xu<sup>1</sup>, Wanlin Guo<sup>2\*</sup>  
and Dapeng Yu<sup>1\*</sup>

<sup>1</sup> State Key Laboratory for Mesoscopic Physics, and Electron Microscopy Laboratory, Department of Physics, 209 Chengfu Road, Peking University, Beijing 100871, China

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We report a significant strain-gradient effect on energy band-gap in bent ZnO microwires with diameter of 0.3~2.5  $\mu\text{m}$ . Strain-gradient breaks the symmetry of local strain effect on energy bands as shown in uniform strained ZnO. Red-shift of the free exciton energy is found to be proportional to the strain-gradient in the tensile and strain-neutral region which could be termed as a flexoelectronic effect, in the elastically bent ZnO wires. We also show theoretically that bending deformation can reduce the energy band-gap of ZnO nanosystems at the density functional level for the first time. The bending deformation induced redistribution of 2p electrons of O is the essential origin for the red-shift, which raise the valance bands and cause remarkable reduction in the band-gap. The revealed strain-gradient effect on band-gap in semiconductors should provide an important new route to band engineering.



Strain-gradient effect on energy bands in bent ZnO Microwires

## Why are Ultrathin Films of Metallic Oxides not Metallic

*Jiandi Zhang\**

*Louisiana State University, USA*

*[jiandiz@lsu.edu](mailto:jiandiz@lsu.edu)*

It has been discovered that many collective phenomena such as high-temperature superconductivity, “colossal” magnetoresistance, and quantum criticality, which do not appear in simple semiconductors, are emergent in complex correlated electron materials (CEMs). Even more surprisingly, many fascinating properties emerge at surfaces, interfaces, and artificial heterostructures of CEMs, the materials beyond mother nature. “The challenge is to understand how such collective phenomena emerge, discover new ones, and to determine which microscopic details are important and essential.”

In contrast with the metallic or even superconducting phenomenon emerging at the interface of two insulating oxides such as  $\text{LaAlO}_3/\text{SrTiO}_3$ , several ultra thin films of metallic oxides exhibit non metallic behavior, challenging our understanding of these materials at interface and under dimensionality control. In this talk, I will discuss this issue: why are ultra thin films of metallic oxides not metallic? I will focus on the ultra thin films of  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  films on  $\text{SrTiO}_3(100)$ , including the lattice structure and critical thickness for metallic properties. Especially, we have found a minimum critical thickness for metallicity as well as a giant response in film transport to the substrate structural phase transition at  $T = 105$  K. These results clearly indicate many new and exciting phenomena can emerge in CEMs through broken symmetry as well as spatial confinement.

\* Supported by US National Science Foundation and US Department of Energy.

Brief Biography:

Dr. Zhang received B.S. and M.S. degrees in physics from the [Nanjing University of Science and Technology](#) in 1982 and the [Chinese Academy of Science](#) in 1986, respectively. He was on the faculty of [Shanghai Jiao Tong University](#) between 1986 and 1989. He received his Ph.D. in physics from [Syracuse University](#) in 1994, spent 3 years as a postdoctoral fellow at [Oak Ridge National laboratory/the University of Tennessee](#) prior to joining the [Florida International University](#) as a faculty member in 1998. Starting from 2009, he became a full professor in physics at [Louisiana State University](#). He is also a visiting professor of the Institute of Physics, Chinese Academy of Science.

## **A Combination of Strain Induced Nanoscale Self-Assembly and Strain Engineered Band Structure**

*Feng Liu*

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Strain induced self-assembly affords one of the most attractive routes to-wards controlled fabrication of low-dimensional nanostructures for the application of next-generation electronic devices. On the other hand, strain is well known for band engineering and has been widely used to improve the performance of Si devices by eliminating the low-mobility bands. In this talk, I will present a unique combination of these two approaches in creating a novel form of hybrid low-dimensional electronic nanostructure: single-element strain superlattice. The evidence that the band gap of Si changes significantly with strain suggests that by alternating regions of strained and unstrained Si, a single-element electronic superlattice (SL) forms with the carrier confinement defined by strain rather than by the chemical differences in conventional compositional SLs. We have mapped out the electronic phase diagram of a one-dimensional pure-silicon strain SL, using first-principles calculations. The pure-Si strain superlattice exhibits a high level of phase tunability, e.g., changing from Type-I to Type-II by tuning the sign of the strain. The theoretical electronic phase diagram rationalizes a recent experimental observation of a strain SL in a Si nanowire and provides general guidance for the fabrication of single-element strain SLs. The unique properties of this class of low-dimensional nanoscale strain SLs, based on new fundamental physical phenomena, may enable a wide range of possible applications.

The work is supported by the Office of Basic Energy Sciences/Materials Sciences and Engineering Division.

## **Multiphase, Multistructure, and Multifunctionality in Interface Engineered Thin Films**

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The modern high-tech research has been explosive in the development of new materials for smart sensors and actuators, sustainable energy harvest and storage devices, self-powered control/sensor systems, driven in parallel by the demands of technology and the inquisitiveness of basic sciences and engineering. These new materials and technology require the integration of materials from different phases, structures, compositions, and physical properties. Interfaces, defined from crystalline/electronic/magnetic phases, structures, and compositions, have become the critical issues in the new materials science and engineering as well as technological development. In particular, complex oxides have demonstrated various important physical properties from pyroelectric to paraelectric to ferroelectric and to piezoelectric, from paramagnetic to diamagnetic to ferromagnetic to ferromagnetic and to diamagnetic, from linear optical to nonlinear optical behavior, and the combinations of these different properties. Integrating complex oxides with multifunctional physical properties directly on semiconductors and/or metallic materials is therefore the dream of new materials research, which may also result in the discovery of new materials properties with controllable functionality and tunability. However, the surface oxidation on semiconductor or/metal surfaces become the road blocks on new multifunctional materials research. The recent successful fabrications of complex oxide ferroelectric BaTiO<sub>3</sub> and BaTiO<sub>3</sub>/SrTiO<sub>3</sub> multilayered structures directly on metallic Ni and semiconductor Si surfaces by using interface engineered nanofabrication technique has opened a new avenue for the integration of complex oxides on semiconductors and structural metallic materials. Also, the discovery of superfast chemical dynamics on highly epitaxial LnBaCo<sub>2</sub>O<sub>5.5</sub> thin film surface is not only fundamental scientific interest but also technological important. These revolutionary developments will have great impact on various modern device developments, such as self-powered structural health monitoring systems, intermediate temperature thin film solid oxide fuel cells, tunable laser systems, and many others. Details will be discussed in the talk.

## **Interface Energy Conversion at the Nanoscale: Insights from Ultrafast Electron Dynamics**

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Nano-structured materials provide wonderful opportunities for generating and utilizing renewable energy sources efficiently, which could lead to novel ways of solving today's energy problem. However, energy conversion mechanisms at the nanoscale remain elusive, especially when the ultrafast energy transfer dynamics is concerned.

In this talk, I will employ the computational tools we recently developed for treating coupled electron-ion dynamics based on time-dependent density functional theory, and explore the mechanisms for ultrafast electron-hole separation at the molecule/semiconductor interface. The resulting timescale and other features agree well with experiments. I will also discuss our recent efforts to establish structure-property relationship for all-organic cyanoacrylic dye solar cells, as well as photosplitting of water using quantum well states of nanoparticles.

## Ultrathin Oxide Films: the “Physics” of Catalysis

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Electronic properties of oxide films quickly converge towards those of the bulk material when studied as a function of atomic layers. We have prepared a variety of oxide films including chromia, niobia, haematite, wuestite, magnetite, alumina, silica, and aluminosilicates. In the case of MgO we have investigated properties as a function of thickness of the film explicitly. In particular, the phononic responses of the film as well as its ability to control charge transfer from the metallic substrate into adsorbates has been investigated. From those observations concepts may be developed to understand the reactivity of thin oxide films under ambient conditions. For thick MgO and CaO films representing the bulk material doping of the films with transition metal and alkali metal atoms and its influence on surface properties has been studied. We report on first results of the preparation of aluminosilicates exhibiting properties of “two-dimensional” zeolites.

## Topological Insulators and Topological Semimetals

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In addition to topological insulator, the topological semimetal is a new non-trivial state with Fermi points in the bulk and Fermi arcs on the surface. In this talk, I will start from our earlier works for  $\text{Bi}_2\text{Se}_3$  family topological insulators, and then move to the recent studies for topological semimetals. I will discuss several possible realizations of those non-trivial states, based on first-principles calculations. In particular, I will address the  $\text{HgCr}_2\text{Se}_4$  and  $\text{Na}_3\text{Bi}$  compounds.

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## **Growth and Si-Layer Intercalation of Centimeter-scale, Highly-ordered, Continuous Graphene on Metal Surfaces for Future Integrated Electronic Devices\***

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Graphene (G), a two-dimensional crystal of carbon atoms arranged in the honeycomb structure, shows extraordinary physical properties such as outstanding electronic mobility, higher than silicon or copper, it is one of the strongest materials found in nature, only comparable to diamond, and at the same time one of the softest, being a unique example of a metallic membrane. Furthermore, the electronic carriers in graphene propagate as a gas of relativistic, chiral, massless Dirac quasi-particles with unusual behavior in the presence of electric and magnetic fields. Because of these and other characteristics, graphene is considered as a serious contender for being the reference material for a post-CMOS technology. Nevertheless, the use of graphene for applications requires mass production of high quality material and also its transfer to insulating substrates. While epitaxial growth in SiC and CVD growth in metal surfaces have seen enormous progress, transfer techniques are still a major challenge and a limiting factor of the material quality. We have developed a new strategy for graphene growth on metallic Ru(0001) followed by silicon-layer intercalation that not only weakens the interaction of graphene with the metal substrate but also retains its superlative properties. This G/Si/Ru architecture, produced by silicon-layer intercalation approach (SIA), was characterized by Raman spectroscopy, scanning tunnelling microscopy/spectroscopy (STM/STS), and angle resolved electron photoemission spectroscopy (ARPES). These experiments have shown the high structural and electronic qualities of this new composite, and the striking differences between this material from graphene obtained by previous methods. The SIA eliminates the need for the graphene transfer and also allows for an atomic control of the distance between the graphene and the metal gate (in this case, the Ru), opening doors for a new generation of graphene-based materials with tailored properties.

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## Chemistry on Nanostructured Templates

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The formation of chemical bonds strongly depends on the spatio-temporal dynamics within an ensemble of starting molecules. Inert chemical systems, such as linear alkane chains are, thus, bad candidates for polymer-forming reactions selectively occurring at ultimate or penultimate positions using conventional chemical approaches in solution or in the gas phase. We found that by using nanostructured surfaces on metallic single crystals, a significant increase of the reaction rate on mild conditions can be obtained, both by the spatial confinement leading to a preferred end-to-end configuration of the molecules, and the catalytic activity of the substrate.

Here, we report that the Au(110) surface which exhibits a one-dimensional (1D) constraint, acts as the platform and heterogeneous catalyst for alkyl C–H activation. The 1.22-nm-wide atomic grooves resulting from the missing-row reconstruction of Au(110)-(1×3) surface efficiently confine the diffusion of adsorbed molecules and constrain the molecules into a 1D pathway, their interactions restricted to neighbouring molecules in the easy-diffusion direction within the atomic channels. Further, we will discuss the use of nanostructured surfaces for the reaction and simultaneous alignment of carbon nano-ribbons over large surfaces areas.

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[www.centech.de](http://www.centech.de)

## **Nanoelectronics Based on Carbon Nanotubes**

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Electronic devices based on carbon nanotubes are among the candidates to eventually replace silicon-based devices for logic applications. Before then, however, nanotube-based radiofrequency transistors could become competitive for high-performance analogue components such as low-noise amplifiers and power amplifiers in wireless systems. Single-walled nanotubes are well suited for use in radiofrequency transistors because they demonstrate near-ballistic electron transport and are expected to have high cut-off frequencies. The one-dimensional (1D) transport leads to a large mean free path (low scattering), high current carrying capability, and low noise within the CNT. Employing CNTs as channels in a transistor has led to predictions of THz performance due to the very low quantum capacitance in a 1D conductor. Here we review progress towards nanotube electronics for radiofrequency applications in terms of device physics, circuit design and the manufacturing challenges.

## STM Investigation of Organic Molecules on Graphene/Ru(0001)

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In the first part of my talk, using epitaxially grown graphene on Ru(0001) as a buffer layer, the intrinsic molecular orbitals of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA), pentacene, and C<sub>60</sub> molecules were imaged by means of scanning tunneling microscope (STM). Combined with density functional theory calculations, our high resolution STM images of the molecules reveal that the graphene layer decouples the individual molecules electronically from the metallic substrate. Our results show that graphene-based moiré pattern can be used as a unique way to probe the intrinsic electronic structures of molecular adsorbates and their interactions.

In the second part, the template-directed assembly of planar pentacene molecules on epitaxial graphene grown on Ru(0001) (G/Ru) has been investigated by means of low-temperature scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. STM experiments find that pentacene adopts a highly selective and dispersed growth mode in the initial stage. By using DFT calculations including van der Waals interactions, we find that the configuration with pentacene adsorbed on fcc regions of G/Ru is the most stable one, which accounts for the selective adsorption at low coverages. Moreover, at high coverages, we have successfully controlled the molecular assembly from amorphous, local ordering, to long-range order by optimizing the deposition rate and substrate temperature.

## Oxides as Templates for Metal Nano-cluster

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Oxides are the ideal templates for growing metallic cluster. Because of their low surface energy most of the metals are growing as islands nucleating at surface defects. To achieve not only self organized- but also self assembled growth the defects where the metal atom nucleate preferentially should show long range order. In this talk two different templates will be discussed. First the four layer thick alumina film which can be grown self limited by oxidation of AlNi<sub>3</sub>(111) and second the surface of Fe<sub>3</sub>O<sub>4</sub>(001). These results are based on STM images with high resolution combined with ab-initio calculations.

The alumina film on AlNi<sub>3</sub>(111) form a nano-mesh with holes down to the substrate and with a distance of 4nm forming a hexagonal super-structure[1]. By filling those holes with few atoms of Pd afterwards almost every metal grow as clusters showing the same hexagonal symmetry. The size of the clusters can be varied between a few atoms up to around 1500 atoms before the cluster they coagulate and form a thin polycrystalline film[2]. We have grown Fe and Co clusters and determined their magnetic properties.

The second template which will be discussed is surface of Fe<sub>3</sub>O<sub>4</sub>(001) which reconstruct in such a way that well ordered single metal atoms can be stabilized on it with remarkable thermal stability[3]. So far Au atoms were grown self-assembled and the usefulness as a model catalyst to measure the reactivity of single Au atoms quantitatively will determined in near future.

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## Direct Growth of Graphene and its Applications in Sensors and Memories

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Growth of large-area and high-quality graphene is important in both fundamental and applied research. Recently, we developed an approach to grow graphene directly on various substrates, making the post-growth transfer process no longer necessary. As-grown nanosized graphene on insulating surfaces has tunable sizes and conductivities and is uniform and continuous at wafer scale. By using a single crystalline substrate which has a similar lattice structure with graphene, we successfully achieved homo- and hetero- epitaxial growth of graphene. The epitaxial graphene is clean, high-quality, and free of interface contaminations, thus provides another material candidate for many physical studies. We also investigated several potential applications for these nanographene films, including using them for piezoresistive strain sensors and resistive randomly accessed memories (RRAM).

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## **Rectifying-based RRAM Crossbar Array for High Density Storage Applications**

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As the semiconductor device continues scaling down, conventional Flash memory is facing more and more bottlenecks and will be very difficult to go through 16 nm node. According to the white paper of ITRS 2010, STT-MRAM and RRAM are thought as the most promising technologies among various emerging non-volatile memory concepts, and are worthy to put additional focuses on research and development to accelerate the progress toward commercialization. In this talk, a brief introduction on RRAM technology will be firstly given and its opportunities & challenges will be discussed. Then, systematic research on Switch Mechanism in Oxide-Electrolyte-Based ReRAM will be introduced.

## **Freestanding nanostructures for three-dimensional nanodevices**

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Free-space nanostructures are the fundamental building blocks of three-dimensional (3D) nanodevices with multi-functionality beyond that achievable by planar devices. Here we developed a reliable technique for the site-specific post-growth geometrical manipulation of freestanding superconducting nanowires using ion-beam irradiation with nanometer-scale resolution to fabricate uniformly shaped and sized clean-surface 3D nanostructures. Such structures could integrate with conventional superconducting quantum interference devices to detect magnetic fields both parallel and normal to the substrate. Property characterizations suggest that our focused-ion-beam technique allows tailoring of freestanding electrical conducting wires and superconducting loops for size and geometry, potentially for novel nanodevices and lab-on-chip experiments.



## **Controllable Magnetic Anisotropies of Epitaxial Fe/Si(111) Films Manipulated by Current Treating**

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We adopted a novel method to tailor the step morphology of the Si(111) substrate, and consequently manipulate the magnetic anisotropy of Fe on it by controlling the direction of treating current. The epitaxial Fe films grown on these Si (111) substrates with different step morphologies were characterized by the scanning tunneling microscope (STM) and rotating magneto-optical Kerr effect (MOKE). The in-plane magnetic hysteresis loops as a function of azimuthal angles demonstrate an alterable uniaxial magnetic anisotropy (UMA) superimposed on the weak six-fold magnetocrystalline anisotropy. The magnetic hysteresis loops simulation based on the coherent rotation model and correlation function calculation were introduced to investigate the magnetic anisotropies. The origin of the controllable UMA was determined to be the long-range dipolar interaction between the spins on the surface.

## **High Pressure Induced Novel Phase Transition in Nanostructured Materials**

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As one of the independent thermodynamic parameters, pressure has been playing an important role in materials and physics. Pressure can be effective in shortening atomic distance, modifying crystalline structures and consequently induce novel high pressure phase which is significantly different from the ambient condition. It is very well established that each material will usually undergo several phase transitions over the pressure range up to Mbar, strongly implying that high pressure could generate plenty of new phases of materials based only on the available ambient compounds. Recently, the phase transformations of nanomaterials under pressure have attracted growing research interest due to the appearance of nanometer scale size effect and the novel high pressure behavior which is hardly discovered in their corresponding bulk samples. Deeply understanding those unusual structures and physical phenomena unveils new aspects of the intrinsic physics of nanomaterials. In this presentation, several examples on high pressure induced novel structural phase transition in typical nanomaterials will be outlined, including high pressure polymerization with combination of nano confinement, unique long range ordered crystal with amorphous building blocks in carbon nanostructured materials as well as the combination of morphology tuning effect in metal oxides, such as pressure induced amorphization and polyamorphism in one dimensional single crystal in metal oxide nanomaterial  $\text{TiO}_2$  nanomaterial and phase transition in well-shaped  $\text{CeO}_2$  nano-octahedrons enclosed by (111) planes. These studies show that high pressure is a powerful tool and provides a new dimension for the study of nanomaterials.

## **Exploring Single-Molecule Electroluminescence through Nanocavity Plasmons**

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Electrically driven single molecular light source is valuable for molecule-based optoelectronic integration and quantum information processing, but still highly demanding due to fluorescence quenching and lack of in-depth understanding on the mechanism. In this talk, I shall demonstrate single molecular electroluminescence originating from intrinsic intramolecular LUMO–HOMO optical transitions of a single porphyrin molecule that is inside the tunnel junction of a scanning tunneling microscope and electronically well-decoupled from the metal substrate. The generation of molecule-specific fluorescence by tunneling electrons is found to depend on two critical factors: one is the electronic decoupling that not only suppresses the fluorescence quenching effects but also creates a double-barrier junction for hole injection; the other is the presence of nanocavity plasmonic fields that spectrally overlap with molecular vibronic transitions and thus enable resonant plasmon-exciton coupling for fluorescence enhancement on both excitation and emission. The injection-type mechanism in organic light emitting diodes (OLED), featuring direct excitation of molecules by injection electrons, has proven inefficient to produce molecular light in the STM tunneling configuration.

## Structure Evolution of $\text{Li}_2\text{MnO}_3$ for Li-ion Batteries

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Layered structure lithium containing transitional metal oxides have been used widely as cathode active materials for Li-ion batteries. It has been well known that only partial of lithium atoms can be extracted out reversibly due to the requirement of lattice stability. Therefore, the reversibly lithium storage capacity is around 140-160 mAh/g (~0.5-0.6 Li). Recently, Thackeray and Johnson proposed composite structures in which a layered  $\text{Li}_2\text{MnO}_3$  component is structurally integrated with either a layered  $\text{LiMO}_2$  component or a spinel  $\text{LiM}_2\text{O}_4$  component (M=Mn, Ni, etc.). The rechargeable capability of this kind of structure can be 250-300 mAh  $\text{g}^{-1}$  (0.8-1.0 Li) by adjusting the element M and the ratio between two components. It has been realized that the enhanced capacity is related to the lithium storage behavior of the parent  $\text{Li}_2\text{MnO}_3$  compound. The interesting points of this material are (1)  $\text{Mn}^{4+}$  in  $\text{Li}_2\text{MnO}_3$  cannot be oxidized further. Therefore, oxygen seems taking the role of charge transfer. This is unusual for most of layered compounds since transitional metal is known as the only active element for charge transfer. (2) One third of lithium atoms occupy 2b sites at the same layer of transition metal. Whether lithium could be extracted out from this layer needs further clarification. Normally, the cation mixing is not favorable for lithium diffusion. (3) Structural evolution after lithium extraction.

Therefore, the variation of electronic state and local structure of  $\text{Li}_2\text{MnO}_3$  are essential issues for understanding the unusual lithium storage mechanism and further optimization of the material.

In this report, with the help of three international teams from BNL, LBNL and University of Tokyo, the structure evolution of  $\text{Li}_2\text{MnO}_3$  before and after delithiation and lithiation has been investigated using synchrotron *in situ/ex situ* XAS and XRD、ABF-STEM、neutron diffraction as well as first principles calculations.

## Electron Transport at the Nanoscale

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Electron transport at the nanoscale is the key to the novel applications of nanomaterials in electronic and energy technologies. Due to the restricted dimensionality, one distinctive character of nano-systems is that the transport properties are critically dependent on the structural details. Therefore, an important requirement for transport research of a specific nanomaterial system is to examine its structures and properties in a coherent manner. As a “nano” version of a four-probe station, ORNL *Four-probe STM* combines STM local imaging and spectroscopy functions with four-point electrical transport capability in a well-controlled sample environment to allow for simultaneous measurements of transport and local structures on the same nanomaterials [1]. In this talk, I will give a brief overview on this unique facility, and then present a few examples to demonstrate how we use this platform to study the electron transport properties and the structure relationships over multiple length scales, from individual atoms, molecules, to nanowires and mesoscopic systems[2-5]. My focus will be on the measurements of individual grain boundary resistance in copper interconnect nanowires [2] and the metal-insulator transitions in self-assembled metal-silicide quantum wires [3, 4]. The goal of this research is to explore the electronic and structural properties on the atomic scale and their impact to the transport functionalities on the mesoscale. This research was sponsored by the Office of Basic Energy Sciences, U.S. Department of Energy.

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## **The Atomic Arrangement in Two-Dimensional Silica – From Crystalline to Vitreous Structures**

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Silica glass has been an extensively studied topic over the last century. Yet, we know little about its atomic-scale structure. In 1932, W. H. Zachariasen postulated that amorphous solids consist of a continuous random network of well defined units [1]. This model has never been verified microscopically with true atomic resolution in real space. Here, we present atomically resolved noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) images of a thin vitreous silica film on Ru(0001) [2]. Characteristic atomic distances and angles are discussed and compared to diffraction data of bulk silica glass. Furthermore, we could resolve the atomic structure of a crystalline—vitreous transition region. The presented silica film is an ideal surface science model to study various properties of glasses.

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## **Probing Nanoscale Phase Separation in Colossal Magnetoresistive Manganites**

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Electronic phase separation and inhomogeneities at the nanoscale have been proven to not only play a key role in the material properties, but also challenge the fundamental concepts of condensed matter physics. In rare-earth doped manganites, the nanoscale phase separation has attracted particular attention because of its relationship with the renowned behavior of the material, colossal magnetoresistance (CMR). Direct observations of the nanoscale phases are usually difficult but necessary to unravel the controversies and unveil the underlying physics in this case. In this talk, we report our recent achievements of direct imaging of the nanoscale phases by using advanced transmission electron microscopic (TEM) techniques correlated with the material property measurements. Based on those results, the relationship between the nanoscale phase and the CMR effect was established, and unexpected magnetic and physical properties of the nanoscale phases were found.

## Understanding Multiple Interactions in Functional Nanostructures of QA Molecules at Metal Surfaces

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The superstructures and self-assembled behavior of a quinacridone derivative with alkyl chains of 16 carbon atoms (QA16C), an organic semiconductor material, on metal surfaces were investigated by the observations of scanning tunneling microscopy and the calculations based on density of function theory. The roles of different molecule–molecule and molecule–substrate interactions for the formation of the nanostructures were fully explored. On Cu(110) surface, QA16C molecules prefer to assemble at submonolayer coverage into two dimensional long-range ordered molecular patterns, in which the lateral alkyl chains exhibit well-ordered flat-lying arrangements. With increasing molecular coverage, the additive QA16C molecules began to form a second layer. As a reason for the layer-by-layer growth on Cu(110), we identify a rigid alignment of the molecule due to the dominate interaction of the molecular backbone with the substrate lattice. While the QA16C molecules on Ag(110) surface, we show how the length and arrangement of carbon side chains of QA16C molecules affect the self-assembled structures and even the mechanical properties of the film in a very subtle manner. It is establish that the involvement of different bond hierarchies, from strong covalent bonding of the backbones to weak van der Waals bonds, results in eight different well-ordered superstructures in the monolayer regime. The detailed insight emerging from this analysis will lead to a much better control in the fabrication of hybrid devices with interfaces between metals and organic molecules.

In collaboration with Prof. Werner A. Hofer, Liverpool University, UK; Prof. Karl-Heinz Ernst, Empa, Swiss; Prof. Yue Wang, Jilin University, China; Prof. Min Ouyang, Maryland University, USA; Stephen J. Pennycook, Oak Ridge National Laboratory, USA.

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## **Molecule-substrate Coupling between Metal Phthalocyanines and Epitaxial Graphene Grown on Ru(0001) and Pt(111)**

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Self-assembly of metal phthalocyanine (MPc) molecules on monolayer graphene (MG) epitaxially grown on Ru(0001) and Pt(111) is investigated by means of low temperature scanning tunneling microscopy. At low coverage, dispersive single molecules, dispersive molecular chains and small patches of Kagome lattice are observed for iron phthalocyanine (FePc), manganese phthalocyanine (MnPc), nickel phthalocyanine (NiPc) and phthalocyanine (H<sub>2</sub>Pc) on MG/Ru(0001), respectively. In contrast, although MG/Pt(111) exhibits various of domains with different moiré patterns and corrugations, FePc molecules always form densely packed two dimensional islands with a square lattice on MG/Pt(111) at submonolayer coverage. The different self-assembling behaviors of MPc molecules on MG/Ru(0001) and MG/Pt(111) originate from a subtle balance between molecule-molecule and molecule-substrate interactions tuned by central metal ions of the MPc molecules and the metal substrates.

# **Xining Part**

## **Nanoparticles as Models for Heterogeneous Catalysts: An Atomic View**

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Model catalyst systems have been prepared by growth of metal nano - aggregates on thin well - ordered oxide films of alumina and silica. These systems lend themselves to structural and morphological characterization via scanning probe microscopies and transmission electron microscopy and bridge to a certain extent the materials gap between metal single crystal studies and the investigation of real catalyst samples. It is possible to infer direct structure - reactivity relations when simple reactions of small molecules are studied. We have applied a variety of surface sensitive techniques including single crystal micro calorimetry, both under ultrahigh vacuum as well as under ambient conditions to relate observations from surface science to those in catalysis under realistic gas pressure conditions. We discuss hydrogenation reactions and CO oxidation and show how the information on model systems can be directly related to realistic systems.

## **A Combination of Strain Induced Nanoscale Self-Assembly and Strain Engineered Band Structure**

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Strain induced self-assembly affords one of the most attractive routes to-wards controlled fabrication of low-dimensional nanostructures for the application of next-generation electronic devices. On the other hand, strain is well known for band engineering and has been widely used to improve the performance of Si devices by eliminating the low-mobility bands. In this talk, I will present a unique combination of these two approaches in creating a novel form of hybrid low-dimensional electronic nanostructure: single-element strain superlattice. The evidence that the band gap of Si changes significantly with strain suggests that by alternating regions of strained and unstrained Si, a single-element electronic superlattice (SL) forms with the carrier confinement defined by strain rather than by the chemical differences in conventional compositional SLs. We have mapped out the electronic phase diagram of a one-dimensional pure-silicon strain SL, using first-principles calculations. The pure-Si strain superlattice exhibits a high level of phase tunability, e.g., changing from Type-I to Type-II by tuning the sign of the strain. The theoretical electronic phase diagram rationalizes a recent experimental observation of a strain SL in a Si nanowire and provides general guidance for the fabrication of single-element strain SLs. The unique properties of this class of low-dimensional nanoscale strain SLs, based on new fundamental physical phenomena, may enable a wide range of possible applications.

The work is supported by the Office of Basic Energy Sciences/Materials Sciences and Engineering Division.

## **The Quantum and Classical Properties of Spins on Surfaces**

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The scanning tunneling microscope has been an extremely successful experimental tool because of its atomic-scale spatial resolution. In recent years this has been combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with microvolt energy resolution. In this talk I will review recent developments in investigating the electronic and magnetic properties of atoms and small clusters of atoms on surfaces. A particular focus will be on the use of magnetic materials for future device applications in the Information Technology industries.

A large enough cluster of magnetic atoms on a surface behaves similar to a macroscopic magnetic particle: its magnetization points along an easy-axis direction in space and magnetization reversal requires sufficient thermal energy to overcome a barrier. How many atoms does it take to create such a magnet? What are the size limits of stable magnetic nanoparticles. Those are important questions for our future technologies.

When the number of atoms in a cluster becomes small quantum tunneling of magnetization can take place and hence quantum mechanics can no longer be ignored but rather takes center stage. Single atoms that are slightly decoupled from conducting substrates behave more like quantum mechanical entities. These quantum systems can be studied with inelastic tunneling spectroscopy, a technique we coined spin-excitation spectroscopy. With this approach it is possible to measure the energy eigenstates of the quantum spin Hamiltonian that describes spins on surfaces with high precision.

## **TiO<sub>2</sub>: Fundamentals, Applications, and Perspectives**

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Research on titanium dioxide, which occurs in multiple surface orientations, is one of the fastest growing areas in Physics and Chemistry, witnessed by an exponential growth in the number of research papers every year. The system is not only a prime candidate for photocatalytic chemistry, it is also the basis of dye-sensitized solar cells, or Graetzel cells. Among many candidates for photocatalysts, TiO<sub>2</sub> is almost the only material suitable for industrial use at present and also probably in the future. This is because TiO<sub>2</sub> has the most efficient photoactivity, the highest stability and the lowest cost. We want to discuss the fundamental properties of the material, explain why it is so versatile, and highlight some recent developments, which shed new light on the actual reaction mechanism on the rutile surface.

## **Dirac Fermion in Strongly-Bounded Graphene Systems**

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It is highly desirable to integrate graphene into existing semiconductor technology, whereby the combined system is thermodynamically stable yet maintaining a Dirac cone at the Fermi level. First principles calculations reveal that certain transition metal (TM) intercalated graphene/SiC(0001), such as the strongly-bounded graphene/intercalated-Mn/SiC, could be such a system. Different from free-standing graphene, however, here the hybridization between graphene and Mn/SiC leads to the formation of a dispersive Dirac cone of primarily TM d characters. The Fermi velocity is half of that of graphene. The corresponding Dirac spectrum remains to be isotropic with transport properties nearly identical to those of free-standing graphene for bias as large as 0.6 V. A simple model Hamiltonian is developed, which can qualitatively account for the physics of the transfer of the Dirac cone from a dispersive system (e.g., graphene) to an originally non-dispersive system (e.g., TM). Work is in collaboration with Yuanchang Li and Wenhui Duan in Tsinghua University.

## Molecules on Moiré Template of Graphene Monolayer Grown on Ru(0001)

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Monolayer graphene was successfully fabricated on 4d transition metal surfaces. The resulting ordered moiré pattern was found to be an ideal template for the formation of ordered nanoclusters and molecules. Using scanning tunneling microscopy (STM) we show the selective adsorption process and assembly of iron phthalocyanine and pentacene molecules with different structural symmetries on a graphene monolayer, epitaxially grown on Ru(0001). The combination of first principles calculations and experimental measurements suggests that the lateral electric dipole is the main driving mechanism for selective adsorption of molecules at fcc regions at low molecular coverage. As increasing the coverage, we observed the formation of regular Kagome lattices that duplicate the lattice of the moiré pattern of monolayer graphene. Varying the central metal ion of the Pc molecule affords Kagome lattices with tunable molecular spins, providing ideal 2D model systems for studying spin frustration. Furthermore, using epitaxially grown graphene on Ru(0001) as a buffer layer, the intrinsic molecular orbitals of PTCDA, pentacene, and C<sub>60</sub> molecules were imaged by means of STM. Combined with density functional theory calculations, our high resolution STM images of the molecules reveal that the graphene layer decouples the individual molecules electronically from the metallic substrate. These findings should be essential in the actual fabrication process. And our results show that graphene-based moiré pattern can be used as a unique way to probe the intrinsic electronic structures of molecular adsorbates and their interactions.

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## **Novel Materials for Nanoscience and Nanotechnology**

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This talk will present our work on carbon nanotubes, graphene nanoribbons and graphene-inorganic hybrid nanomaterials. Biological applications of carbon nanotubes will be discussed including a new fluorescence imaging method in the so called NIR-II region in the spectral window of 1000-1400nm. NIR fluorescence enhancement of carbon nanotubes and organic fluorophores will be presented on a novel plasmonic substrate for 3D molecular tracking and biological detection. I will then talk about graphene nanoribbons, including several methods recently developed in our lab to form high quality graphene nanoribbons with narrow widths and smooth edges. Lastly, I will talk about our recent work on making inorganic nanoparticles and nanocrystals on graphene sheets for energy storage and electrocatalytic applications.

## **Multiphase, Multistructure, and Multifunctionality in Interface Engineered Thin Films**

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The modern high-tech research has been explosive in the development of new materials for smart sensors and actuators, sustainable energy harvest and storage devices, self-powered control/sensor systems, driven in parallel by the demands of technology and the inquisitiveness of basic sciences and engineering. These new materials and technology require the integration of materials from different phases, structures, compositions, and physical properties. Interfaces, defined from crystalline/electronic/magnetic phases, structures, and compositions, have become the critical issues in the new materials science and engineering as well as technological development. In particular, complex oxides have demonstrated various important physical properties from pyroelectric to paraelectric to ferroelectric and to piezoelectric, from paramagnetic to diamagnetic to ferromagnetic to ferromagnetic and to diamagnetic, from linear optical to nonlinear optical behavior, and the combinations of these different properties. Integrating complex oxides with multifunctional physical properties directly on semiconductors and/or metallic materials is therefore the dream of new materials research, which may also result in the discovery of new materials properties with controllable functionality and tunability. However, the surface oxidation on semiconductor or/metal surfaces become the road blocks on new multifunctional materials research. The recent successful fabrications of complex oxide ferroelectric  $\text{BaTiO}_3$  and  $\text{BaTiO}_3/\text{SrTiO}_3$  multilayered structures directly on metallic Ni and semiconductor Si surfaces by using interface engineered nanofabrication technique has opened a new avenue for the integration of complex oxides on semiconductors and structural metallic materials. Also, the discovery of superfast chemical dynamics on highly epitaxial  $\text{LnBaCo}_2\text{O}_{5.5}$  thin film surface is not only fundamental scientific interest but also technological important. These revolutionary developments will have great impact on various modern device developments, such as self-powered structural health monitoring systems, intermediate temperature thin film solid oxide fuel cells, tunable laser systems, and many others. Details will be discussed in the talk.

## Spin Shuttles

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Fullerenes may incorporate atoms with an open electron shell. This implies a well defined and chemically protected electron spin system. The recent finding that single dysprosium ions inside a C<sub>80</sub> carbon cage display at 2 K 4f electron spin orientation lifetimes of several hours will be presented [1]. This opens perspectives for the use of these DySc<sub>2</sub>N@C<sub>80</sub> molecules as a spin shuttle on surfaces.

[1] An Endohedral Single-Molecule Magnet with Long Relaxation Times: DySc<sub>2</sub>N@C<sub>80</sub>, Westerström *et al.*, J. Am. Chem. Soc. (2012) DOI: 10.1021/ja301044p

## Oxides as Templates for Metal Nano-cluster

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Oxides are the ideal templates for growing metallic cluster. Because of their low surface energy most of the metals are growing as islands nucleating at surface defects. To achieve not only self organized- but also self assembled growth the defects where the metal atom nucleate preferentially should show long range order. In this talk two different templates will be discussed. First the four layer thick alumina film which can be grown self limited by oxidation of AlNi<sub>3</sub>(111) and second the surface of Fe<sub>3</sub>O<sub>4</sub>(001). These results are based on STM images with high resolution combined with ab-initio calculations.

The alumina film on AlNi<sub>3</sub>(111) form a nano-mesh with holes down to the substrate and with a distance of 4nm forming a hexagonal super-structure[1]. By filling those holes with few atoms of Pd afterwards almost every metal grow as clusters showing the same hexagonal symmetry. The size of the clusters can be varied between a few atoms up to around 1500 atoms before the cluster they coagulate and form a thin polycrystalline film[2]. We have grown Fe and Co clusters and determined their magnetic properties.

The second template which will be discussed is surface of Fe<sub>3</sub>O<sub>4</sub>(001) which reconstruct in such a way that well ordered single metal atoms can be stabilized on it with remarkable thermal stability[3]. So far Au atoms were grown self-assembled and the usefulness as a model catalyst to measure the reactivity of single Au atoms quantitatively will determined in near future.

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## Electron Transport at the Nanoscale

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Electron transport at the nanoscale is the key to the novel applications of nanomaterials in electronic and energy technologies. Due to the restricted dimensionality, one distinctive character of nano-systems is that the transport properties are critically dependent on the structural details. Therefore, an important requirement for transport research of a specific nanomaterial system is to examine its structures and properties in a coherent manner. As a “nano” version of a four-probe station, ORNL *Four-probe STM* combines STM local imaging and spectroscopy functions with four-point electrical transport capability in a well-controlled sample environment to allow for simultaneous measurements of transport and local structures on the same nanomaterials [1]. In this talk, I will give a brief overview on this unique facility, and then present a few examples to demonstrate how we use this platform to study the electron transport properties and the structure relationships over multiple length scales, from individual atoms, molecules, to nanowires and mesoscopic systems[2-5]. My focus will be on the measurements of individual grain boundary resistance in copper interconnect nanowires [2] and the metal-insulator transitions in self-assembled metal-silicide quantum wires [3, 4]. The goal of this research is to explore the electronic and structural properties on the atomic scale and their impact to the transport functionalities on the mesoscale. This research was sponsored by the Office of Basic Energy Sciences, U.S. Department of Energy.

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## Quantitative Surface Analysis and Generation of Complex Biomimetic Structures by AFM

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While the imaging capabilities of techniques such as STM, SFM, and near field optics (SNOM) etc. dominated the application of these methods at their early development stages, the physics of probe-sample interactions, and the quantitative nanoanalysis of elastic, electronic and magnetic surface and transport properties became recently of increasing interest. Force spectroscopy allows us, for example, to gain information about folding and unfolding processes of individual protein molecules and other biologically relevant systems. Beyond that we can do now quantitative imaging of the potential landscape of surfaces at the atomic scale thus getting valuable data for the understanding of the atomic scale mechanisms underlying, e.g. friction- and wear processes. These techniques may also open the pathway for non-destructive *chemical* surface-analytical investigations at the atomic scale.

Non energetic writing techniques which became feasible by DIPen Lithography allows us to write chemical diverse small structures for the interaction with biological systems such as biological cells. Recent developments and perspectives of these techniques will be discussed.

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[www.uni-muenster.de/Physik/PI/Fuchs](http://www.uni-muenster.de/Physik/PI/Fuchs)

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## **Probing Nanoscale Phase Separation in Colossal Magnetoresistive Manganites**

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Electronic phase separation and inhomogeneities at the nanoscale have been proven to not only play a key role in the material properties, but also challenge the fundamental concepts of condensed matter physics. In rare-earth doped manganites, the nanoscale phase separation has attracted particular attention because of its relationship with the renowned behavior of the material, colossal magnetoresistance (CMR). Direct observations of the nanoscale phases are usually difficult but necessary to unravel the controversies and unveil the underlying physics in this case. In this talk, we report our recent achievements of direct imaging of the nanoscale phases by using advanced transmission electron microscopic (TEM) techniques correlated with the material property measurements. Based on those results, the relationship between the nanoscale phase and the CMR effect was established, and unexpected magnetic and physical properties of the nanoscale phases were found.

## **Graphene epitaxy on Ru(0001): a template for supramolecular nano-architectures**

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Graphene, a true two-dimensional material, has attracted intensive interest due to its fascinating properties, e.g., room temperature quantum Hall effect, massless Dirac fermions, and electronic spin transport. Epitaxial graphene overlayer grown on transition-metal substrates often exhibits moiré pattern due to the lattice mismatch between graphene overlayer and substrate. In this talk we demonstrate that the moiré pattern of single layer graphene epitaxially grown on Ru(0001) can act as a wonderful template to guide the formation of a variety of supramolecular nano-architectures.