



Workshop USTC/CEA 2009 October, 5 to 8th

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Nearly Free Electron States in Gated Graphene Nanoribbon Superlattices

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Abstract: An extremely clean one dimensional electron system is designed based on graphene nanoribbon superlattices. Upon electron doping, nearly free electron states distributed in the vacuum area between two graphene nanoribbons can be occupied and act as an ideal ballistic transport channel. The proposed structure is thus a very good field effect transistor with high mobility and on-off ratio. It is also an ideal system to study electron correlation in one dimensional, as a pure electron system without atomic scattering.



BIOGRAPHY

Jinlong Yang, Changjiang professor of physical chemistry, dean of the School of Chemistry and Material Sciences of USTC, received his Ph.D. in condensed matter physics from USTC in 1991. His research interests focus on developing first principles methods and their applications on clusters, nano structures, solid materials, surfaces, and interfaces.



metal

Dynamics and Statistics of Electron Transport in Single Molecules

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Abstract:

A hybrid computational approach that combines molecular dynamics simulations with first principles calculations to study electron transport property of a single molecular junction in aqueous electrolyte will be introduced. It allows providing statistic distribution of molecular conductance in solution at different temperatures and to produce conductance histograms that can be directly compared with experiments. It is found that the experimentally observed temperature dependent conductance can be attributed to the thermal effect on hydrogen bonding network around the molecule and be described by the radial distribution of water molecules with their hydrogen-bonded atoms in the molecule. The statistic behavior of the conductance is shown to be very sensitive to the external gate electric field and multi-peaks distributions of the conductance can even occur in a single molecular junction.

I will describe a few recent studies on single molecular conductance switches. One of the examples is the observation of conductance switching with tuneable frequency as a result of mechanical oscillation of a single N-H bond in the molecule [2]. A dynamic model is developed to describe the observed non-integer power law dependence of switching rate for different molecular systems [2,3,4]. Molecular switching and NDR effect generated by the electric field induced dipole change of the molecule will also be discussed [5].

A new computational scheme, named as a central insertion scheme (CIS), for electronic structure of nanostructures will be presented [6]. With efficient parallel implementation, electronic structures of very large systems, up to 150000 electrons, can be routinely obtained at different density functional theory levels. In comparison with conventional computational methods, CIS provides results with the same high accuracy but requires only a fraction of computational time. Applications of this scheme for carbon nanotubes, nanodiamond, DNA, and polymers will be given.

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BIOGRAPHY

Yi Luo, Professor in Theoretical Chemistry at both USTC and Royal Institute of Technology (KTH), Sweden. He obtained his PhD in computational physics in 1996 in Linkoping University, Sweden. Before moving to KTH in 2000, he worked as an assistant professor in Stockholm University. He has published 220 papers in international leading journals in the fields of quantum chemistry, molecular photonics, molecular electronics and synchrotron radiation based X-ray spectroscopies.

New Synergic-assembly Strategy towards Three-dimensional Hollow Hierarchical Nanostructures

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Abstract:

The construction of nano-architectures has been the hot-topic subject for the nanomaterial-synthesis field. The nano-architectures have the special coupling or synergic property advantages that are resulted from the combination effect of the ordered building block units, leading to their unique properties compared with the mussy individual nano-units themselves, which are of great interest for the next-generation nano-architecture design. This present review describes a novel way to grow and assemble the 3D hollow hierarchical nanostructures, with the utilization of the synergic effects of hollowing process from the self-produced templates and the highly anisotropic growth of nan-ounits of the target materials in one-pot reaction. In this process, the building block nano-units spontaneously in-situ form owing to their highly anisotropic internal structure, while the self-produced templates act as the supporter and growth-direction guidance for the in-situ formed nan-ounits. Therefore, the whole assembly process is simple, controllable and without the complicated manipulations.

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(5) Z.Q. Li, Y. Ding, Y. J. Xiong, Q. Yang, and Y. Xie*, Chem. Commun., 2005, 918.

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BIOGRAPHY

Yi Xie, received her BS in Xiamen University (1988) and her Ph. D in University of Science and Technology of China (1996). She is now a Principal Investigator (PI) of Department of Nanomaterials and Nanochemistry, Hefei National Laboratory for Physical Sciences at Microscale and a full professor of Department of Chemistry, University of Science and Technology of China. She is also a recipient of many awards, including China Young Scientist Award (2002), China Young Female Scientist Award (2006), Chinese Academy of Sciences-Bayer Young Scientist Award (2003), the Cheung Kong Scholar (2000). Her research interests are in solid state and materials chemistry.

New Synthetic Strategies for Unique Functional Inorganic Nanostructures, Hybrid Nanomaterials and Their Applications

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Abstract:

Development of new synthetic strategies for unique functional nanostructures has attracted a lot of attention. Herein, we will report several facile synthetic protocols for one-pot controlled synthesis of several kinds of unique inorganic nanomaterials and hybrids under mild solution conditions, in which simple organic molecules, surfactant or low molecular weight polymers have been used. The key roles of additive/surfactant as well as the synergistic effects of growing nanostructures and an organic template have been studied. These unique nanostructures include magnetic nanorings, conducting nanocables and nanotubes, polymer@Ag nanospheres, and new hybrid semiconducting nanobelts/nanowires, and new carbon-based nanostructures. The properties of these unique nanostructures and their potential applications will be discussed.

References

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BIOGRAPHY

Shu-Hong Yu, received his B.Sc. degree from Hefei University of Technology in 1988, and his PhD from University of Science and Technology of China (USTC) in 1998. He worked in Tokyo Institute of Technology as a JSPS Research Fellow from 1999 to 2001. He was awarded an AvH Fellowship (2001-2002) in Max Planck Institute of Colloids and Interfaces, Germany. He became a faculty member in School of Chemistry & Materials as a full professor in 2002. Currently, he is leading the Division of Nanomaterials and Chemistry, Hefei National Laboratory for Physical Sciences at Microscale, and also acting as the vice dean of the School of Chemistry & Materials, USTC. He was appointed as Group Leader of the Partner Group of the Max Planck



Society and the Chinese Academy of Sciences. He has authored and co-authored more than 187 refereed journal publications, 9 invited book chapters, and 6 patent. He serves as an associate editor for international journal Material Research Bulletin (Elsevier), and the advisory board members of journals CrystEngComm (RSC), Nano Research (Tsinghua Press, Springer), Current Nanoscience, Chinese Science Bulletin (specially invited editor), and Chinese Journal of Inorganic Chemistry. His research interests are focused on synthesis of inorganic nanostructures and new inorganic-organic hybrid materials, polymer controlled crystallization and biomineralization, carbon materials and energy storage.

Controllable fabrication and optical properties of ZnO one dimensional nanostructure

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Abstract:

ZnO one dimensional (1-D) nanostructure, regarded as one of the most promising inorganic functional nanomaterials, possess many extraordinary and fascinating properties, a tremendous upsurge studies has thus been reported on the preparation and properties of ZnO 1-D nanostructures in recent years. Whether its morphology, size, microstructure, composition, orientation as well as the optical properties can be prepared in a controllable way is also the prerequisite of putting ZnO-based nanodevices in practice. However, despite the remarkable progresses that have been made in the fabrication of ZnO 1-D nanostructures, most of the previously reported methods are still lack of control. Besides, the studies as well as the understandings on how to efficiently tailor the optical properties of ZnO 1-D nanostructures are still quite limited. In this report, the efforts will be focused on the fabrication control and optical properties tailoring of ZnO 1-D nanostructures with vapor phase synthesis process. We first demonstrate how to fabricate controllably the well-aligned, single-crystalline ZnO nanoarrays with different tip-shapes and discuss the morphology dependence for their optical, transport and field-emission properties. With spatially-resolved cathodoluminescence spectra, we will also present the results for the strong size and surface effect on the luminescence of individual ZnO nanorods. At last, we will repot briefly the effort to fabricate the highly-oriented, hierarchical nanobelt-nanopillar arrays from self-assembled ternary oxide Zn-In-O.

BIOGRAPHY

Xiaoping Wang, received his B. S. in 1987, M. S. in 1990, and Ph. D. in 2001 in University of Science and Technology of China. He is now as a full professor of Physics in the University of Science and Technology of China and the vice director of Hefei National laboratory for the Physical Sciences at the Microscale. His current research focuses on the nanostructures and nanodevices. He has authored and co-authored more than 60 refereed journal publications and 10 patents.

New phenomena in molecular electroluminescence from tunnel junctions

Zhenchao Dong, Jianguo Hou

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Abstract:

Control of radiative properties of functional molecules near metals is a key issue in nanooptics, important for light manipulation at the nanoscale and the development of molecular plasmonic devices. Up to date, light emissions in these systems are restricted by Kasha's rule and Franck-Condon principle, namely the fluorescence is always from the lowest vibronic level of the excited state. Here we report an experimental study of electrically driven molecular fluorescence of porphyrins in a highly confined nanogap constructed by a metal tip and metal substrate. Striking high-energy hot luminescence directly from highly excited vibrational states is observed, which breaks the vibrational relaxation limit and is a result of strong resonant coupling between electric-field induced nanogap plasmon and the molecular vibronic transition. Our observations demonstrate that, the strong near-fields of local nanogap plasmons behave like a strong coherent optical source with tunable energy and can be used to actively control the radiative channels of molecular emitters via intense resonance enhancement on both excitation and emission.

BIOGRAPHY

Zhen-Chao Dong is currently a Professor in Hefei National Laboratory for Physical Sciences at Microscale and University of Science and Technology of China. His research interest is in the field of single molecule optoelectronics and nanoplasmonics, particularly on tunneling electron induced fluorescence from single molecules and quantum tuning of photonic states at the molecular scale.

Dong obtained a BS degree in Chemistry from Sichuan University (1983), a MS degree from Xiamen University (1987), and a PhD degree from Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences (CAS, 1990).



After his postdoctoral research at Ames Laboratory/Iowa State University, he moved to National Institute for Materials Science (NIMS, Japan) in 1996 and was promoted to a senior researcher in 1998 and a sub-theme leader in 2001. In 2004, he joined the University of Science and Technology of China as a full professor. He is the author of over 100 publications, among them five first-author papers were published in Phys. Rev. Lett.(1), J. Am. Chem. Soc. (3), and Angew. Chem. Int. Ed. (1), respectively, plus many others in Phys. Rev. B, Appl. Phys. Lett., Surf. Sci., Adv. Mater., Inorg. Chem., etc. His papers have been cited more than 1000 times.

Charge inhomogeneity, fluctuation and soliton in atomic wire arrays

Changgan Zeng

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Abstract:

Similar to strongly-correlated materials, some low-dimensional systems may also show striking cooperative phenomena due to enhanced charge, spin, lattice coupling. We investigate the atomic wire array system based on In/Si(111) at atomic scale by adopting scanning tunneling microscopy. Charge inhomogeneity and fluctuation are observed far below previously reported transition temperature (from high temperature x1 phase to low temperature x2 phase). Novel phases are revealed and the bias voltage can tune the periodic modulation along the wire direction. Defect and electric field seem critical to understand these effects. Soliton behavior at atomic scale is observed in the insulating x2 structure. The atomic structure of soliton, interaction between solitons, and their motion are studied systematically. Manipulation of the soliton is also realized by applying pulsed voltage.

BIOGRAPHY

Changgan Zeng

Education and research experiences

- 1993-1997: B.S., Department of Modern Physics, University of Science and Technology of China
- 1997-2002: Ph.D., Structure Research Lab., University of Science and Technology of China
- 2001.12-2002.2: RA, Department of Physics, Muenster University, Germany
- 2002-2007: Postdoc, Department of Physics and Astronomy, University of Tennessee, US
- 2007-present: Professor, Hefei National Laboratory for Physical Sciences at Microscale, Department of Physics, University of Science and Technology of China

Research interests

• Construction, characterization and manipulation of collective orders in low-dimensional structures

Detecting and controlling electronic and spin states at a single molecular scale

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Abstract:

The exploration on the bonding interaction, charge and spin transport, optoelectronic transformation, and information carriers for quantum communication in molecular scale systems may provide insights into the nature and principle of quantum manipulation, enable us to understand the operational mechanism of molecular electronic and optoelectronic devices, and thus lay foundation for next-generation quantum information and energy technologies.

We demonstrated in joint experimental and theoretical study how one can alter electron transport behavior of a single melamine molecule adsorbed on Cu(100) surface by performing a sequence of elegantly devised and well controlled single molecular chemical processes.

We also demonstrated that the spin state and magnetism of single phthalocyanine molecules on Au(111) can be tuned by pruning the hydrogen atoms in the molecules using a scanning tunneling microscope. A scheme to build up multiple Kondo centers with the help of a single molecular template is proposed. It is demonstrated that by taking advantage of unique structure property of cobalt phthalocyanine (CoPc) molecule, one can place Co atoms at each end of the benzene rings to form Kondo resonance with 1, 2, 3, and 4 centers, respectively, as verified by scanning tunneling microscopy. It is shown that the Kondo centers are spatially separated but strongly coupled through hybridization with delocalized molecular states, leading to large variation of Kondo temperature. It is found that the degree of coupling among different Kondo centers can be largely enhanced by increasing symmetry of the molecular complex.

BIOGRAPHY

Bing Wang, Professor of physics in USTC. He obtained his Ph.D degree in condensed matter physics in 1995 in USTC. After his postdoctoral research at Hong Kong University of Science and Technology (1997-1999), he came back USTC. His current study interests focus on the electronic transport of low dimensional nanostructures and surface science. He has published 70 papers in international leading journals.

Adiabatic Factoring Algorithm and its experimental realization

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Abstract:

Secure communication based on cryptographic systems such as RSA is widely used in daily life. The security of these systems is based on the fact that no efficient algorithm is known for large-integer factorization on classical computers. But quantum computer has shown the potential to break this system with a moderate time when Peter Shor proposed his famous factoring algorithm. While Shor's algorithm is based on the traditional quantum circuit model, we are interested in the factoring schemes by another quantum computing architecture – the adiabatic quantum computation. The new adiabatic factoring algorithm shows some advantages towards Shor's algorithm. By this new algorithm, we firstly factored the number 21 on liquid NMR quantum computer last year. Recently, we improve this record to an even large number 143 which is the largest number been factored by quantum algorithms so far.

BIOGRAPHY

Jiangfeng Du Prof. Dr. Jiangfeng Du from the University of Science & Technology of China (USTC), *Yangzi* Professor (Ministry of Education, P.R.C.) at Hefei National Laboratory for Physical Sciences at Microscale, USTC. He specializes in the experimental realization of Quantum Computing by using magnetic resonance technologies, and some related fundamental issues of Quantum Physics.

Experimental quantum communication

Zengbing Chen

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Abstract:

Experimental quantum communication is one of the main topics in Division of Quantum Physics and Quantum Information in HFNL. In this talk I summarize the main progresses on experimental quantum communication carried out in our Division. Our progresses include the experimental realizations of the first robust quantum repeater node, practical quantum cryptography and quantum network, and free-space quantum communication.

BIOGRAPHY

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Experience

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