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The Second Stig Lundqvist Research Conference on the Advancing Frontiers in Condensed Matter Physics:

"Non-Conventional Systems and New Directions"

2 - 6 July 2001

Miramare - Trieste, Italy

Directors:	*D. Awschalom, University of California at Santa Barbara* *E. Burstein, University of Pennsylvania, Philadelphia* *G. Scoles, Princeton University, Princeton*
Local Organizer:	*E. Tosatti, SISSA and ICTP, Trieste*

Co-sponsored by:

- the Office of Naval Research, ONR, Arlington, VA, USA
- the National Science Foundation, NSF, Washington, DC, USA
- the Conselho Nacional de Desenvolvimento Cientifico e Tecnologico, CNPq, Brazil
- the Scuola Internazionale Superiore di Studi Avanzati, SISSA, Trieste, Italy

FINAL PROGRAMME AND ABSTRACTS

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PREFACE

This workbook contains the Programme and the Abstracts of the Invited Talks and Posters that were presented at the Second Stig Lundqvist Research Conference on the Advancing Frontiers of Condensed Matter Physics which was held under the main sponsorship of the Abdus Salam International Centre for Theoretical Physics (ICTP) from 2 July 2001 to 6 July 2001. The specific theme of the Conference was "Non-Conventional Systems and New Directions". Its focus was on major developments during the last few years in "soft" and "hard" condensed matter science and on the overlap between physical science and biology. The goal was to bring together scientists who are playing key roles in these areas to discuss their ongoing research and to assess the progress that is being made in their respective fields. The Conference was aimed at the exploration of new opportunities in condensed matter science, ranging from the manipulation of matter at the atomic scale to interfaces involving inorganic and biological systems.

The Stig Lundqvist Research Conference on the Advancing Frontiers of Condensed Matter Physics was established as a biannual Conference by Prof. Miguel Virasoro, Director of the Abdus Salam International Centre for Theoretical Physics, "in recognition of the outstanding role which Stig Lundqvist played at ICTP". The first Stig Lundqvist Research Conference on the Advancing Frontiers of Condensed Matter Physics which had as its theme "Quantum Phases in Electron Systems of Low Dimensions" was held from 26 July 1999 to 29 July 1999. Stig Lundqvist was Professor of Theoretical Physics at Chalmers University of Technology in Göteborg, Sweden from 1964 to 1990. He was a member of the Nobel Prize Committee for Physics from 1972 to 1985 and its Chairman from 1980 to 1985. At ICTP he served as Chairman of the Scientific Council from 1983 to 1992, and as head of the Condensed Matter Physics Programme. The series of Adriatico Research Conferences that were started in 1985 is his brainchild. He was awarded the Dirac Medal of the ICTP in 1990 and on his 70th birthday in 1995, he was designated ICTP Distinguished Condensed Matter Scientist, Emeritus. As a condensed matter scientist, Stig Lundqvist had a deep interest in the continued exciting theoretical, conceptual and experimental progress of the field. It is therefore most appropriate that the biannual Stig Lundqvist Research Conferences have as their theme "The Advancing Frontiers in Condensed Matter Physics".

As Directors of this Second Stig Lundqvist Research Conference, we are grateful to the ICTP for making this forum available to the condensed matter community. We are indebted to the Office of Naval Research (ONR) and the National Science Foundation (NSF) of the USA, the Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq) of Brazil and the Scuola Internazionale Superiore di Studi Avanzati (SISSA) of Italy for their co-sponsorship of the Conference. We also wish to express our deep appreciation to Prof. Yu Lu, Head of Condensed

Matter Section at ICTP, for his advice and guidance in organizing the Conference, and to Nicoletta Ivanissevich, the Conference Secretary, for her patience and help in solving administrative problems that arose before and during the Conference.

David Awschalom, Professor of Physics, University of California at Santa Barbara
Elias Burstein, Mary Amanda Wood Professor of Physics, Emeritus, University of Pennsylvania
Giacinto Scoles, Donner Professor of Science, Princeton University
Erio Tosatti, Professor of Physics, SISSA and ICTP, Trieste

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FINAL PROGRAMME

All lectures were held in the Adriatico Guest House - Kastler Lecture Hall

Monday, 2 July

09:00 - 10:30	**Registration**
10:30 - 12:00	Time open for administrative matters
	Opening Session Chairperson: **E. Burstein**
14:00	Welcome **M. Virasoro**, Director of the Abdus Salam I.C.T.P., Trieste **Yu Lu**, The Abdus Salam I.C.T.P., Trieste
14:15	Introductory Remarks **D. Awschalom**, University of California, Santa Barbara
14:45 - 15:45	**B. Batlogg**, ETH Zürich *Molecular organic crystals: A new playground for many-body physics*
15:45 - 16:15	Coffee break
16:15 - 17:15	**J. Joannopoulos**, MIT, Cambridge *Novel light phenomena in photonic crystals*
17:15 - 18:15	**K. Takayanagi**, Tokyo Institute of Technology, Yokohama *Conductance of nano-scale quantum point contact*

Tuesday, 3 July

Morning Session

Chairperson: **D. Awschalom**

09:00 - 10:00	**D. Loss**, University of Basel *Electron spins in quantum dots for quantum computing*
10:00 - 11:00	**H. Ohno**, Tohoku University, Sendai *Ferromagnetic/nonmagnetic III-V semiconductor structures*
11:00 - 11:30	Coffee break
11:30 - 12:30	**D. H. Cobden**, University of Warwick *Kondo physics in carbon nanotube quantum dots*

Afternoon Session

Chairperson: **J. Joannopoulos**

14:30 - 15:30	**G. Abstreiter**, TU München *Optical properties of single semiconductor quantum dots*
15:30 - 16:10	**G. Salis**, University of California, Santa Barbara *All optical NMR in nanostructures*
16:10 - 16:40	Coffee break

Chairperson: **M. P. Das**

16:40 - 17:20	**H. Schön**, Bell Labs, Lucent Technologies, Murray Hill *Lasing in molecular organic single crystals*
17:20 - 18:00	**A. Yodh**, University of Pennsylvania, Philadelphia *Entropic forces and self-assembly of microstructures in suspensions*
18:00 - 18:50	**P. Pincus**, University of California, Santa Barbara *Coulombic effects in soft condensed matter*

Wednesday, 4 July

	Morning Session
	Chairperson: **M. Cardona**
09:00 - 10:00	**K. H. Rieder**, Freie Universität Berlin *Physics and chemistry with single atoms and molecules using the STM*
10:00 - 11:00	**M. Persson**, Chalmers University, Göteborg *Spectroscopy and chemical manipulation a the spatial limit*
11:00 - 11:30	Coffee break
11:30 - 12:30	**M. Salmeron**, Lawrence Berkeley National Laboratory, Berkeley *On the microscopic mechanism of friction*
	Afternoon Session
	Chairperson: **G. Scoles**
14:30 - 15:20	**B. Persson,** IFF, FZ Jülich *Sliding friction*
15:20 - 16:10	**G.-Y. Liu**, Wayne State University, Detroit *Molecular manipulation on surfaces*
16:10 - 16:40	Coffee break
	Chairperson: **P. Fazekas**
16:40 - 17:30	**A. Lucas**, University of Namur *Diffraction by molecular helices: from DNA to carbon nanotubes*
17:30 - 18:20	**E. Mele**, University of Pennsylvania, Philadelphia *Quantum geometric phases in molecular nanotubes*
20:00 - 22:30	**Poster Session**

Thursday, 5 July

Morning session

Chairperson: **E. Burstein**

09:00 - 10:00	**D.H. Vanderbilt,** Rutgers University, Piscataway *Role of compositional order and disorder in complex perovskites*
10:00 - 11:00	**C.B. Murray**, IBM, T. J. Watson Research Center, Yorktown Heights *Self-organization of nanocrystal superlattices: building with artificial atoms*
11:00 - 11:30	Coffee break
11:30 - 12:30	**R. Car,** Princeton University *Designing enzyme mimics: electron transfer in oxomanganese porphyrins*

Afternoon Session

Chairperson: **D. Vanderbilt**

14:30 - 15:10	**B. Noheda,** Brookhaven National Laboratory, Upton *High piezoelectric response in complex ferroelectric oxides*
15:10 - 16:00	**A.M. Belcher,** University of Texas, Austin *Evolving biomolecular control of semiconductor and magnetic nanostructures*
16:00 - 16:30	Coffee break

Chairperson: **G. P. Brivio**

16:30 - 17:20	**J. Hone**, California Institute of Technology, Pasadena *Nanoelectromechanical systems*
17:20 - 18:20	**A. Pinczuk**, Columbia University, New York *Milli-Kelvin spectroscopy of electron quantum liquids in semiconductors*

Friday, 6 July

Closing Session

Chairperson: **Yu Lu**

09:00 - 10:00 **E. Tosatti,** S.I.S.S.A. & The Abdus Salam I.C.T.P., Trieste
String tension, structure and stability of tip-suspended gold, silver and platinum nanowires

10:00 - 10:30 Coffee break

10:30 - 11:30 **M. Parrinello**, Max-Planck-Institut, Stuttgart & ETH, Zürich
Ab-initio simulation of chemical processes in realistic environments

11:30 - 12:30 **G. Scoles**, Princeton University
Unusual physical and chemical processes in superfluid helium nanodroplets

ABSTRACTS OF TALKS

The optical properties of single semiconductor quantum dots

Gerhard Abstreiter

Walter Schottky Institut, Techn. Univ. Munich, D-85748 Garching

Semiconductor quantum dots have attracted a lot of interest recently due to their possible applications in optoelectronics, nanoelectronics, quantum information processing and chemical/biological sensing. Conventional optical spectra, probing many dots at the same time, are broadened inhomogeneous due to variations in size, shape, and composition. Sharp spectral lines in absorption and emission, which are important for most of the novel applications mentioned above, are only observed when individual quantum dots are studied. The work on single dot spectroscopy started nearly a decade ago [1-7]. In the past 4 years nearly hundred papers appeared in the literature, reporting on various aspects of single dot spectroscopy demonstrating the vastly growing interest in this field of research [8]. Spectroscopy with high spatial resolution concomitant with separation of dots in space or in transition energy has been used to study the population of single or coupled dots populated with one or a few electron-hole pairs. Photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE) with and without applied magnetic field allows the identification of ground-state and excited electronic levels as well as phonon-assisted processes. The formation of biexcitons (2 electrons and 2 holes in the dot) and filling of higher states is observed in PL with increasing excitation power [2, 9]. In special electrically tunable semiconductor structures it is also possible to study charged excitons and to obtain a well defined controllable population of the dots [10]. In magnetic fields characteristic features with respect to the spin population and spin dynamics are observed, which may be of interest to future quantum information processing. Under resonance excitation a spectrally sharp and tunable photocurrent is obtained in reverse biased single dot photodiodes [11].

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[10] F. Findeis et al., Phys. Rev. **B63**, 121309R (2001)
[11] F. Findeis, M. Baier, E. Beham, A. Zrenner, and G. Abstreiter, Appl. Phys. Letters **78**, 2958 (2001)

Molecular organic crystals: a new playground for many-body physics

Bertram Batlogg [a b], J. Hendrik Schön [a] and Christian Kloc [a]
[a] *Bell Labs, Lucent Technologies, Murray Hill, NJ 07974, USA*
[b] *ETH Solid State Physics Laboratory, CH-8093 Zürich, Switzerland*

High quality organic molecular crystals are a new and productive area to study many-body interactions in solids. The main advantage is the flexibility to induce charges by the field-effect technique, leading to the continuous transformation of a highly insulating material into a metal. As the charge carrier density is varied by many orders of magnitude one encounters a multitude of physical phenomena of current interest. In the talk we will emphasize the dilute and the concentrated limit. The electron-electron interaction is found to be an order of magnitude stronger than in other semiconductors with the same carrier density, giving rise to stable quantum Hall states up to relatively high temperature. In addition, the interaction of charge carriers with lattice vibrations leads to a pronounced temperature-induced enhancement of the effective mass. In the high-density limit, i.e. when the charge carrier concentration varies from a tenth to several per molecule, we find different ground states. In particular we discuss the ground states as the Fermi level is shifted from below half-filling of the valence band to above half-filling of the conduction band, following e.g. the superconducting transition temperature. Comparisons will be made between the different materials, and factors influencing superconductivity will be discussed.

J. H. Schön, Ch. Kloc, B. Batlogg, Phys. Rev. Letters, 86, 3843-3846 (2001)
J. H. Schön, Ch. Kloc, H. Y. Hwang, and B. Batlogg, Science 292,252-254 (2001)
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Evolving Biomolecular Control of Semiconductor and Magnetic Nanostructures

Angela M. Belcher
The Department of Chemistry and Biochemistry, The Texas Materials Institute,
The Institute of Cellular and Molecular Biology
The University of Texas at Austin

Biological systems have a unique ability to control crystal structure, phase, orientation and nanostructural regularity of inorganic materials. We are currently investigating the principles of natural biological molecular recognition in materials and developing new methods to pattern useful non-biological electronic and magnetic materials on new length scales. A peptide combinatorial approach has been employed to identify proteins that select for and specifically bind to inorganic structures such as semiconductor wafers and semiconductor and magnetic nanoparticles. This approach utilizes the inherent self-organizing, highly selective properties of biologically derived molecules. We are currently investigating peptide recognition and interaction with III-V and II-VI semiconductor materials and magnetic materials. We have selected peptides that can specifically bind to and discriminate zinc-blende III-V semiconductor surfaces. These peptides show crystal face specificity and are being used to organize nanoparticles heterostructures. We have also selected peptides that can nucleate and control phase, particle diameter and aspect ratio of II-VI semiconductor nanoparticles. These peptides are being used to grow nanoparticles and nanowires of specific crystallographic structure and orientation. Using these molecular interactions and specific nanoparticles we are organizing organic/inorganic hybrid materials into supramolecular architectures.

Designing Enzyme Mimics: Electron Transfer in Oxomanganese Porphyrins

Roberto Car
Princeton University, Department of Chemistry and Princeton Materials Institute

(work done in collaboration with Filippo De Angelis, Ning Jin and John T. Groves Department of Chemistry, Princeton University, Princeton, NJ 08544)

Metal porphyrins are a common molecular motif in a wide range of biological and catalytic processes involving oxygen activation and transfer, such as for instance those occuring in the respiration cycle. Understanding the correlation of electronic structure and reactivity of metal porphyrins is essential to design synthetic catalytic mimics of bio-enzymes. Here we consider in particular the case of oxo-manganese (V) porphyrins in electron transfer reactions which have been recently characterized experimentally. Based on Density-Functional-Theory calculations we explain the strong pH dependence of the rate constant, increasing 4 orders of magnitude from pH 9 to 5 and the different reactive behavior observed for a series of meso-substituted porphyrins. Significantely, theory and experiment agree that a more electron deficient porphyrin translates into a more stable electrophilic catalyst, in marked contradiction of traditional reactivity correlations.

KONDO PHYSICS IN CARBON NANOTUBE QUANTUM DOTS

David H. Cobden*, Department of Physics, University of Warwick, UK

The physics of quantum dots is central to the description of mesoscopic and molecular-scale electronic devices. Its importance is largely in how it overlaps condensed matter and atomic physics and expands their boundaries. An example of how quantum dots make accessible new realms of physics is seen in the emergence of the Kondo effect as a key feature of their low temperature transport properties when the contacts are strongly coupled [1]. Besides displaying the standard Kondo signatures long known from bulk materials, such as logarithmic temperature dependences, quantum dots make it possible for the first time to study Kondo-like physics controllably out of equilibrium, and with an electronic spectrum which can be continuously tuned by gate voltage or magnetic field. Although most studies have been made in semiconductor structures, quantum dots can also form in very different host materials, such as individual single-wall carbon nanotubes [2]. It is now established that nanotube quantum dots can act as nearly ideal one-dimensional electron boxes. The one-dimensional bands, the different energy scales, and the absence of orbital shifts and spin-orbit coupling, offer a powerful comparison and contrast with the situation in two- and three-dimensional semiconductor dots. In nanotube dots we find [3] regular even-odd alternation of the Kondo behaviour with electron number, low-temperature saturation at the unitary limit at zero magnetic field, new Kondo resonances induced at level crossings in a magnetic field, and bias dependences consistent with new nonequilibrium theories. Finally, it is interesting to note that while semiconductor dots are normally embedded in a crystal, molecular quantum dots can be much more physically accessible, for instance being suspended in vacuum, and it should therefore be possible to probe and couple to them in a much wider variety of ways.

Work done in collaboration with Jesper Nygard, Niels Bohr Institute, Copenhagen, Denmark.

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Novel light phenomena in photonic crystals

J. D. Joannopoulos

In an effort to further the progress of high-density integration and system performance, scientists are now turning to light (or optical photons) instead of electrons as the information carrier. Photons have several advantages over the electron, including the ability to carry a larger amount of information and to interact much more weakly with the host system which helps reduce energy losses. Recently, a new class of artificially designed dielectric materials known as *photonic crystals*, offer a new and significantly better mechanism for confining and propagating light. The difference lies in the concept of a *photonic band gap* - the optical analogue of the electronic band gap in semiconductors. For wavelengths in the band gap, light can be perfectly confined at defects in the otherwise crystalline lattice. Thus point defects can act as microcavities, line defects as microwaveguides, and planar defects as perfectly reflecting mirrors. This provides a new dimension in oneís ability to control and manipulate light. Prof. Joannopoulos will present an overview of this new field including recent exciting developments demonstrating how photonic crystals can be used to make light do things that have never been possible before. These include the possibility of guiding optical light in air and around very sharp (zero radius of curvature) waveguide bends without incurring any losses1-3, the ability to induce photon-photon transitions without the need for non-linear materials4, the ability to control spontaneous emission by many orders of magnitude (either enhance or inhibit)1, and the ability to achieve perfect tunneling through localized states in channel dropping configurations.5

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4. M. Skorobogatiy and J.D. Joannopoulos, Rigid Vibrations of a Photonic Crystal and Induced Inter-Band Transitions, *Phys. Rev. B* **61**, 5293 (2000).

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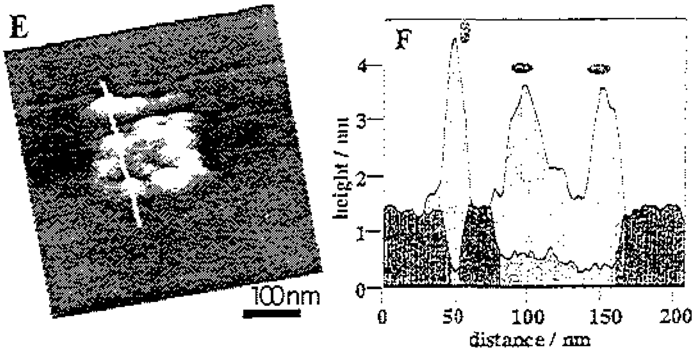
Molecular Manipulation on Surfaces

Gang-yu Liu
Department of Chemistry, Wayne State University, Detroit, MI 48202, USA

Our research aims at developing new engineering protocols to pattern biomolecules on surfaces with nanometer to molecular precision. Patterning proteins or other bioreceptors on surfaces is the key step in the fabrication of biosensors and biochips. While microfabrication techniques allow production of protein or DNA patterns with micrometer dimension, selectively patterning and immobilizing proteins with molecular precision remains an obstacle. This presentation will introduce new nanofabrication methods using scanning probe microscopy such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Discussions will include the fabrication principles, procedures and various examples of nanostructures, one of which is shown in the figure below.[1]

Compared with other microfabrication methods, scanning probe lithography allows more precise control of the size and geometry of the nanopatterns. Resolution better than 1 nm can be routinely obtained. Multiple component features are fabricated and nanostructures can be quickly changed, modified, and characterized *in situ*.[1,2] The fundamental information obtained from these investigations should serve as a useful guide in nanofabrication for biosensors, biochips and new biomaterials. The engineering methodology developed here shall benefit the development of ultra-small biosensors and biochips by increasing the density of receptor elements, improving detection limits, and controlling the reactivity of the receptor elements by engineering them with molecular precision.

Nanopatterns of lysozyme



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Electron Spins in Quantum Dots for Quantum Computing

Daniel Loss
Department of Physics
University of Basel, Switzerland

If the states of electron spins in solids can be created, manipulated, and measured at the single-quantum level, an entirely new form of information processing, quantum computing and quantum communication, will be possible [1]. I review [2] our proposed spin-quantum dot architecture for a quantum computer, thereby indicating a variety of first generation nanostructures, as well as magnetic and electrical measurements which should be considered. I will discuss a spin filter and spin detection mechanism [3]
at the single-spin level which can be used for read-in and read-out in
conventional as well as in quantum computer gates. Addressing the feasibility of quantum communication with entangled electrons [2,5,6] I discuss electronic Einstein-Podolsky-Rosen pairs produced by an ``Andreev entangler"[7,8] and show that the spin entanglement of two electrons (in a Fermi sea) can be detected in transport and noise measurements in mesoscopic systems [5,6].

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Diffraction by Molecular Helices: from DNA to Carbon Nanotubes

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ABSTRACT

The ubiquitous and beautiful helical organization of the biological world at the molecular level of DNA [1], protein alpha-helices [2], etc... as well as at the mesoscopic scale of viruses [3], cellular fibers [4], etc... has been investigated mostly by diffraction methods. Recently the Carbon nanotubes were discovered [5] by high resolution electron microscopy and their detailed atomic structure has again been determined by electron diffraction [5], [6]. In this lecture I will use optical simulation experiments (the optical transform method) to explain just how X-ray fiber diffraction and electron diffraction have been used to reveal the helical arrangements of B-DNA [7], Carbon nanotubes [8] and the microtubules of the animal cell.

The audience will have the opportunity to take part, hands on, in the optical simulation experiments.

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Quantum Geometric Phases in Molecular Nanotubes

E.J. Mele
Department of Physics
University of Pennsylvania

The electronic properties of single wall nanotubes of carbon and of boron nitride are controlled by the size and geometric structure of the nanotube lattices.
In this talk we focus on some novel quantum geometric effects that arise in these structures.
For carbon nanotubes, the gap structure and the response to elastic mechanical deformation are unified in a single theory that introduces these effects through an effective vector potential seen by pi electrons propagating on the curved surface. For III-V BN nanotubes the theory predicts a spontaneous ground state electric polarization arises as an intrinsic quantum geometric effect in the tube geometry.
Consequences for the piezo electric and photogalvanic properties of these structures will be discussed. Finally we will discuss an extension of the theory to new electronic effects in BN nanotori.

Self-organization of of nanocrystal superlattices: Building with artificial atoms

Christopher B. Murray

Synthetic chemistry allows to production nanometer scale structures which are uniform size to + or - one lattice constant while controlling crystal shape, structure and surface passivation. We combine a high temperature solution phase synthesis with size selective processing techniques to produce organically passivated magnetic and nanocrystals with size distributions less than 5%. These nanocrystals then form the basis for a combined structural and magnetic study of the evolution nanocrystal properties with size. These monodisperse nanocrystals self-organize during controlled evaporation to produce 2D and 3D superlattices (colloidal crystals, opals). The nanocrystals resemble "artificial atoms" sitting on regular close-packed superlattice sites, each separated by a selected organic spacer. The inter-particle spacing can be varied from intimate contact up to ~40Å separation. The superlattices retain and enhance many of the desirable mesoscopic properties of individual nanocrystals and permit the first systematic investigation of new collective phenomena. Our goal is to study the properties of both the dispersed nanocrystals and assemblies as all major structural parameters are varied (composition, size, and spacing). Procedures have been developed for Co, Ni, and FePt magnetic nanocrystals as well as for II-VI and IV-VI semiconductor nanocrystals (Quantum Dots). Recent explorations of magnetic recording and the transport phenomena in the magnetic nanocrystal superlattices will be discussed along with efforts to engineer the optical properties of the quantum dots. Progress in the development of techniques to pattern nanocrystal superlattices, which will be essential to the fabrication of devices incorporating these molecular-scale building blocks will also be high-lighted.

HIGH PIEZOELECTRIC RESPONSE IN COMPLEX FERROELECTRIC OXIDES

*B. Noheda**
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Solid solutions of lead zirconate and lead titanate, $PbZr_{1-x}Ti_xO_3$ (PZT), show excellent electromechanical properties and are the base for all current piezoelectric devices, including sonars, ultrasound machines, hydrophones, micropositioners, etc., as well as for the new generation of smart materials and structures with integrated sensing and actuating functions. When an electric field is applied, these ceramic materials can deform as much as 0.15% for compositions close to the boundary between their tetragonal and rhombohedral phases, a nearly vertical line in the T-x phase diagram generally called "morphotropic phase boundary" (MPB). However, despite of its wide use, the reason for the extraordinary electromechanical response of PZT has been an enigma for about 50 years. More recently, other solid solutions with similar phase diagrams, $Pb(Mg_{1/3}Nb_{2/3})_{1-x}Ti_xO_3$ (PMNT) and $Pb(Zn_{1/3}Nb_{2/3})_{1-x}Ti_xO_3$ (PZNT), have shown even more outstanding properties, with electromechanical deformations of 1.7% and piezoelectric coefficients five times larger than those of PZT[1], pointing to a revolution in the actuator industry.

In the last three years, high-resolution x-ray diffraction experiments on PZT, PZNT and PMNT have shown that a third phase with lower symmetry (monoclinic or orthorhombic) is always present around the MPB[2]. Moreover, studies done with an electric field applied *in-situ* have demonstrated that the monoclinic phase can be induced in these materials by the application of an electric field[3]. The monoclinic symmetry allows the polarization vector to rotate within the monoclinic plane, what is not possible in the classic piezoelectric materials such as quartz, in which the field can only produce elongation along a symmetry axis. This extra degree of freedom (the rotation of the polarization) is the actual cause for the high piezoelectricity in these oxides. These results are in very good agreement with recent first-principles[4] and phenomenological[5] studies.

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*In collaboration with D.E. Cox, G. Shirane, L.E. Cross, R. Guo, S-E. Park and Z. Ye.

Ferromagnetic/Nonmagnetic III-V Semiconductor Structures

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I review our study on ferromagnetic/nonmagnetic heterostructures based on III-V compounds. Hole-induced ferromagnetism in Mn doped GaAs and InAs [1] allows us to explore spin-dependent phenomena in semiconductor heterostructures and opens possibilities of controlling semiconducting properties through spins and vice versa. A mean-field theory based on exchange between carrier spin and Mn spin is capable of explaining the ferromagnetic transition temperatures, strain-dependent easy axis, and peculiar temperature dependence of magnetic circular dicrhoism [2], when realistic band structure is incorporated using a $k \cdot p$ approximation [3]. Magnetic/nonmagnetic trilayer structures based on III-V's have been shown to exhibit spin-dependent scattering, tunnel magnetoresistance as well as interlayer coupling due to the carrier polarization [4]. Electrical spin injection across a ferromagnetic/nonmagnetic semiconductor heterojunction and into an InGaAs quantum well (QW) has been demonstrated using ferromagnetic (Ga,Mn)As as a source of spin polarized carriers [5]. Gate control of ferromagnetism has also been demonstrated recently [6]. By the use of magnetic/nonmagnetic semiconductor heterostructures, we are beginning to learn how to control and utilize the spin degree of freedom in semiconductors. Routes to room temperature ferromagnetism will also be discussed.

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Ab-initio simulation of chemical processes in realistic environments

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The conventional approach to the theoretical study of chemical reactions has been to study the reactivity of atoms and molecules in isolation. However, practical chemistry takes place in solution, at surfaces and in general under conditions of strong interaction with the surrounding environment. Furthermore, thermodynamic parameters strongly influence the way and the speed at which a reaction proceeds. *Ab-initio* molecular dynamics offers a unique tool for studying and understanding chemical processes as they normally take place in the laboratory or in industry. In fact, it combines chemical accuracy with the possibility of studying the influence of the environment and the effect of temperature and pressure. One limiting factor, however, is the time scale over which most chemical reactions take place, which far exceeds the simulation time scale. We shall present a method that is able to generate classical trajectories with fixed initial and final boundary conditions. Our method is based on the minimization of a suitably defined action. In combination with the path sampling method of Chandler *et al.*, it promises to be a powerful tool for solving the time scale problem in the study of chemical reactions.

Sliding Friction

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ABSTRACT

I present a broad overview of sliding friction. I discuss boundary lubrication, and emphasize the fundamental role of the atomic corrugation of the confining solid walls on the squeezing and sliding of molecular thin lubrication films. The properties of atomic and molecular lubricants confined between two approaching surfaces are investigated by molecular dynamics and kinetic Monte Carlo calculations. In the limit of thin interfaces, the lubricant atoms form well defined layers, whose number decreases in discontinuous stepswith increasing applied pressure. These transitions occur easily and completely for unpinned lubricant films, while they are sluggish and incomplete in the case of strong pinning. Before the transition, an intermediate phase arises, which facilitates the thinning of the lubricant. Lateral sliding of the surfaces enhances the thinning rate. I also show that for two-dimensional (2D) liquid-like layers, the squeeze-out exhibit instabilities which may result in trapped islands of lubrication molecules, as observed in recent experiments. I consider the sliding of boundary lubricated surfaces and discuss the nature of the lubrication film during the transition from stick to slip.
Finally, I discuss rubber friction and a new theory of contact mechanics.

- Sliding Friction: Physical Principles and Applications, Second (expanded) Edition (Springer, Heidelberg, June 2000).
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Spectroscopy and Chemical Manipulation at the Spatial Limit

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The motions of individual atoms and molecules adsorbed on metal surfaces, such as vibration[1], rotation [2], diffusion [3], bond dissociation [4] and formation [5], are effectively probed by a low temperature scanning tunneling microscope (STM). In addition to its imaging capabilities, manipulation, spectroscopic characterization, and chemical modification can be carried out with sub-Ångstrom resolution. By probing individual atoms and molecules, intrinsic properties are obtained, which are free from ensemble averaging and environmental effects. Other unique applications of the low temperature scanning tunneling microscope include the study of the molecular conductivity and spatially resolved magnetism and superconductivity.

In this talk we will present a few illustrative examples of these unique capabilities of the STM, discuss some of these examples in view of current theory [4,6,7], and present some theoretical challenges. In particular we will stress the important role of vibrational inelastic tunneling in controlling the individual atomic motions and in atomic-scale characterization of adsorbed species.

On the one hand, the theory is based on simple, qualitative models that identify the key mechanisms and concepts. On the other hand, density functional calculations of chemisorbed molecules provide detailed quantitative understanding of inelastic tunneling and a basis for a development of new concepts.

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Coulombic Effects in Soft Condensed Matter

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We discuss electrostatic phenomena in soft condensed matter systems in the context of biomolecular forces. In particular, we shall emphasize the interplay between Coulombic interactions and statistical mechanics to encourage e.g. DNA condensation, by provoking attractive forces between like charged surfaces.

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Milli-Kelvin spectroscopy of electron quantum liquids in semiconductors

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Since its introduction, in 1978-79, the inelastic light scattering method has been used extensively to study collective excitations of low-dimensional electron systems in semiconductor quantum structures. Our recent work demonstrates light scattering studies of collective quasiparticle excitations of electron quantum fluids in the semiconductor structures.[1-3]

Electron liquid states in artificial quantum structures are striking manifestations of fundamental interactions. The intriguing states emerge in low-disorder electron systems at high magnetic fields or at ultra-low densities. Inelastic light scattering studies of 2D quantum fluids are carried out at temperatures that may be lower than 100mK degrees, while the electron densities can be as low as 10^9 cm^{-2}. Impact of condensation of low-dimensional electron systems into novel quantum states is seen in the unique behaviors of characteristic low-energy excitation modes. The recent work reviewed in this presentation creates new venues to probe the energy level structure of composite fermion quasiparticles. These experiments offer key tests of current theories of electron liquid states in the quantum Hall regime.

(*) In collaboration with B.S. Dennis, I. Dujovne, M.A. Eriksson, C. Hirjibehedin, M. Kang, V. Pellegrini, A.S. Plaut, L.N. Pfeiffer and K.W. West.

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Physics and chemistry with single atoms and molecules using the STM

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The scanning tunneling microscope (STM) has been developed in recent years from an instrument capable of imaging surfaces with atomic resolution to an operative tool with which surfaces can be modified on nanometer and even atomic scale. The STM-provides several parameters by which atoms and molecules at (and in) surfaces can be influenced: The tip/sample forces, the tunneling current and the field between tip and surface [1].

For the technique of "soft" lateral manipulation, in which particles can be moved in a very precise manner on the surface, only the forces have to be applied. Different manipulation modes like pushing, pulling and sliding can be experimentally distinguished by tracing tip-height cutves during movement. Upon movement of native substrate atoms across step edges exchange processes appear to be important [2]. For controlled vertical manipulation, in which a particle is transferred from the surface to the tip and vice versa, also field and current effects play a role. We show that deliberate transfer of molecules to the tip leads to chemical contrast in imaging and improved resolution [1,3]. Examples of the buildup and in-situ characterization of nanostructures fabricated from single atoms and small molecules are presented [3]. The utility of lateral manipulation in physical investigations like the determination of long range lateral interactions on metal surfaces is demonstrated [4]. We show also that parts of larger molecules can be influenced mechanically in a precise way leading to extreme differences in electrical behaviour thus opening up the possibility of a mechanical switch based on single molecules [5]. Effects due to the tunneling current are decisive for the dissociation and association of molecules: The artificial induction of all steps of a complex chemical reaction employing single molecules is demonstrated with the technologically important Ullman reaction (see figure): (i) Preparation of the reactands (phenyl) by dissociation of the parent molecules (iodobezene), (ii) bringing together two reactands by lateral manipulation and (iii) welding the reactands together to the final product (biphenyl) by electron bombardment [6]. Prospects to extend the STM-manipulation techniques to thin layers of insulating materials on metal substrates leading to new surprising restructuring effects are discussed [7].

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All-optical Nuclear Magnetic Resonance in Semiconductor Quantum Structures

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The hyperfine interaction between the spin of quantum-confined electrons and nuclei is employed to optically address local nuclear moments [1,2]. Periodic optical excitation of the electron system in the presence of a magnetic field is shown to resonantly tip the dynamically polarized nuclear spin. By optically monitoring the nuclear dynamics with time-resolved electron-spin Larmor magnetometry, we study such nuclear resonances in a 7.5 nm wide single GaAs quantum well at liquid helium temperatures. Depolarization of he nuclear spin at the full and half conventional resonance fields, as well as quadrupolar splittings of the resonance peaks, are attributed to Dm = 1 and Dm = 2 transitions within the Zeeman-split nuclear levels. Amplitude modulation of the periodic laser excitation reveals sidebands in the spectra. For Dm = 2 transitions, hyperfine coupling is not the dominant tipping mechanism, as suggested from the absence of sidebands in the case of electron-spin modulation. Comparing resonances induced by optically injected electrons with and without spin polarization reveals that the charge, and not the spin of the electron induces Dm = 2 transitions, which is explained by coupling to the nuclear electric quadrupole moment.

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On the microscopic mechanisms of friction

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Proximal probes (Atomic Force Microscopy and Surface Forces Apparatus), and Spectroscopies (Sum Frequency Generation), are used to study the molecular nature of friction in single asperity contacts. Energy dissipation during friction can be decomposed into contributions of elementary processes that can be identified by suitable experiments. I will illustrate some of these concepts in the case of single crystal surfaces with and without monolayers of self-assembled molecules. In particular I will show the contribution of molecular distortions, collective tilts and point defect production to the overall energy budget of rubbing interfaces.

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4. Generation of defects in model lubricant monolayers and their contribution to energy dissipation in friction.
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Lasing in molecular organic single crystals

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Stimulated emission in organic materials has been known for more than 30 years. However, lasing induced by electrical exitation has been found to be very difficult to achieved. Some reasons for that have been identified in the low charge carrier mobilities, unbalanced and inefficient injection of charge carriers, as well as charge-induced absorption in the region of optical gain. The use of high-quality molecular crystals can solve these problems. Mobilities in the range of 1 cm2/Vs can be obtained for electrons as well as holes at room temperature. Due to the delocalized character of the charge carriers charge-induced absorption can be minimized. Moreover, the use of fiel-effect electrodes rather than conventional etal electrode can provide good injection

properties. This led to the demonstration of the first organic solid state injection laser [1,2]. Device design and ways towards thin film structures will be discussed.

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UNUSUAL PHYSICAL AND CHEMICAL PROCESSES IN SUPERFLUID HELIUM NANODROPLETS

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Doping an intense beam of superfluid helium nanodroplets with atoms or molecules, followed by probing their properties by means of laser spectroscopy, allows for the study of superfluidity on the nanoscale and of chemical reactions at previously untried low temperatures. Does a molecule, rotating in a superfluid, behave like a macroscopic body under the same conditions, or is there new information to be gathered probing superfluidity at the molecular level? What can we learn about many-body interactions studying the far-from-equilibrium clusters of atoms and molecules that can be synthesized at these very low temperatures? Are there any practical applications in sight? In this talk I will try to give an at least partial answer to these questions and to give a flavour of this expanding field of research.

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Conductance of Nano-Scale Quantum Point Contact

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Conductance and structure of metal quantum point contact (QPC) was studied by an STM aided UHV transmission electron microscopy simultaneously. Since we observe STM tip and specimen surface simultaneously, the motion of the scanning tip and the surface strain induced by the tip became visible. Making a contact between gold tip and substrate forms gold nanowire. Withdrawal of the tip results in diameter change of the nanowire in steps and conductance quantization in the unit of $2e^2/h$, where e is electron charge and h, Planck constant1). Step-wise change in their structure suggests a certain "magic" structure for the gold nanowire. Surprisingly, the gold nanowires have multi-shell structure2), like carbon nano-tubes. The finest tube that we have found is a single wall tube with six atomic rows, which coil around the tube axis. The conductance of the tube has not been measured, and theoretical prediction of the stability and conductance is quite interesting. Particularly interrupting is a suspended gold atom strand: The strand has not broken until its atomic spacing reaches to 0.4nm1,3).

Making a hyperbolic constriction of gold contacts, we observe no conductance change in steps while withdrawal of the gold STM tip. As soon as the contact changes into a wire of a regular diameter, the conductance takes quantized value4). Thus, quantum states at the contact become well defined for the wire length of the order of Fermi wavelength. Beyond conductance quantization of gold nanowires (multi-shell effect) and alkali-metal nanowires (shell effect), conductance of disordered material such as liquid and amorphous semiconductor is an interesting issue. Some recent experimental results and explanations will be presented.

Topics presented are (1) EM observation of STM tip and surface, (2) and (3) TEM of gold contact with and without conductance quantization, (4) Multi-shell magic metal nanowires, (5) gold atom strand, (6) conductance of liquid nanowire: beyond QPC.

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String Tension, Structure and Stability of Tip-Suspended Gold, Silver and Platinum Nanowires(*)

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The mechanism stabilizing the magic chiral nanowires, recently realized and imaged in gold between (110) tips [1], is under scrutiny [2], also in view of the possibility that other metals could show the same phenomenon. We present a theory of tip-suspended nanowires, very recently proposed and tested for gold [3], and use it to examine the possibility of magic nanowires in silver, and in platinum.[4]
A tip-suspended nanowire in grand canonical equilibrium with the tips, with atoms freely exchanged between the two, is described by a generalized string tension. The string tension is generally positive and decreases with decreasing nanowire radius. At finite temperature, the wire will release its tension through flow of atoms from the wire to the tips, causing a spontaneous and progressive thinning [5,6].
At the end of this process the wire eventually breaks and the string tension vanishes. A local minimum of the tension versus radius signifiesa relatively long lived metastable nanowire with that radius. We thus propose that such local string tension minima should correspond to the magic nanowires.

The zero-temperature string tension can be calculated from first principles. First a set of trial nanowire structures is built using e.g., a Lennard-Jones potential , and/or an empirical many body potential if available. Candidate optimal structures are refined by full electronic structure calculations. From the wire total energy and length, and the bulk metal cohesive energy providing an estimate of the tip chemical potential, the grand canonical energy per unit length, which is precisely the string tension, is directly obtained.

We find that the thinnest non-monatomic gold nanowire with lowest tension -- which we may call the (7,3)-1 wire, because it consists of one central atomic strand, surrounded by a seven-strand tube with helicity three -- is in striking agreement with the structure proposed by Kondo and Takayanagi. [1] Parallel calculations for platinum suggest a rather similar scenario to that of gold, whereas in silver the (7,3)-1 wire is not so stable. Thicker nanowires pose a heavier computational problem, and have not been calculated yet. However, some of the reported regularities, in particular the chiralities, can already be qualitatively understood based on our picture.

The microscopic electronic mechanism leading to stabilize these peculiar nanowire geometries for the noble metals can be pursued in terms of electronic structure. We find for gold that electronic shell closing can be ruled out; comparison of gold, silver, and platinum supports instead a close connection with surface reconstruction.

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Role of compositional order and disorder in complex perovskite ferroelectrics

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Perovskite ferroelectrics and related materials are of growing importance for their widespread use as piezoelectric actuators and transducers and in non-volatile memory applications. The materials of most interest for applications are cubic ABO_3 perovskites with Pb on the A site and a mixture of cations (typically Ti, Zr, Nb, etc.) on the B site. The presence of this compositional complexity on the B site presents both challenges and opportunities for *ab-initio* theory.

In the first part of the talk I will focus on our development of a detailed theoretical description [1] of the structural, dielectric, and piezoelectric properties of $Pb(Zr_{1-x}Ti_x)O_3$ (PZT), the best-known material of this class. In view of the decades of previous study, the recent discovery [2] of a monoclinic phase in an important region of the x-T phase diagram of PZT is rather remarkable. I will outline how it is possible to construct a theory that proceeds from *ab-initio* calculations on a database of compositionally ordered structures at zero-temperature, to a successful description of the disordered finite-temperature system. Our theory not only provides an excellent description of the unusual piezoelectric properties of this material, but also explains how these are intimately connected to the proximity of the monoclinic phase.

In the latter part of the talk I will discuss the opportunities provided by the possibility of intentional control of the compositional order in complex perovskites. In recent work [3], we have shown that such control may lead to a qualitatively new kind of piezoelectric material in which the inversion symmetry of the ferroelectric double-well potential is broken by an intentional layering sequence imposed during atomic-layer epitaxial growth. This opens the way to a new class of materials with tunable ferroelectric and piezoelectric properties.

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Entropic forces and self-assembly of microstructures in suspensions

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The addition of small macromolecules (particles) to a suspension of large particles causes an entropic attraction to arise between the large particles. The origin of this attractive force is an increase in volume (i.e. entropy) available to the smaller particles that arises when the large particles are moved close together [1]. We review this effect and experimentally explore its manifestations near walls and wall-structures [2], and in semi-dilute solutions of polymeric DNA [3]. Light force microscopies to measure colloidal particle interactions are introduced and experimentally demonstrated in some of these systems [3]. Finally, entropically driven nucleation and assembly on grating surface templates is demonstrated [4].

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ABSTRACTS OF POSTERS

Magnetic edge states and their transport in a one dimensional electron gas in the presence of a nonhomogeneous magnetic field

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The spectrum of magnetic edge states and their transport properties in the presence of a perpendicular non-homogeneous magnetic field in a quantum wire formed by a parabolic confining potential are obtained. Systems are studied where the magnetic field exhibits a discontinuous jump in the transverse direction and changes its sign, strength, and both sign and strength at the magnetic interface. The energy spectra and wave functions of these systems, the corresponding group velocities along the interface and the particle average positions normal to the interface are calculated.

The resistance of the quantum wire in the presence of such a magnetic interface is obtained both in the ballistic and the diffusive regimes as a function of the Fermi energy and of the homogeneous background magnetic field. The results are compared with those for the case of a homogeneous field.

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SURFACE STRESS AND THE 3x3 DISTORTION OF Sn/Ge(111)

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The 3x3 distortion found experimentally and later confirmed theoretically on Sn/Ge(111) sqrt(3)xsqrt(3) has been tentatively described as a charge-density-wave, or as a band Jahn-Teller distortion, originating from the half-filled surface state in the band gap. We present physical arguments, supported by detailed electronic structure calculations of the distorted and undistorted surface, which suggest a different mechanism.
Calculations indicate that upon 3x3 distortion the electron kinetic energy decreases by a large amount of 206 meV/adatom, only partly compensated by a corresponding potential energy increase of 197 meV/adatom. This is exactly opposite to what is expected for a charge-density-wave, or a band Jahn-Teller distortion, where potential energy drives the energy lowering, and kinetic energy rises, to compensate part of that.
We checked that this is the case with direct dimerization calculations in a hydrogen atom chain, and in polyacetylene. Therefore the physics of these CDW systems should be different from that of Sn/Ge(111), which remains unexplained.

One possibility presently being investigated is an excessive compressive surface stress in the undistorted sqrt(3)xsqrt(3) surface. In the hydrogen chain cartoon, we indeed find that a compression would result in an excess of electron kinetic energy, and that this excess could be released by, e.g, a zig-zag distortion. Similarly, if the top third of monolayer of Sn adatoms was excessively tight, it might release energy -- largely kinetic -- by the 3x3 buckling distortion.
We are presently investigating this mechanism, and spelling out its experimental consequences.

Enhanced surface resistivity induced by 3d magnetic adatoms

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The resistivity of a thin metal film is very sensitive to surface conditions when temperature is as low as 10 K. Defects such as steps and adsorbates scatter conduction electrons impinging on the surface diffusively, leading to an increase in resistivity compared to the clean surface. It was only recently that a microscopic expression of the surface resistivity was derived for the case of semi-infinite metals [1,2]. The only input for this formula is the wave function (or Green's function) of electrons at the Fermi energy, appropriate for the semi-infinite geometry. In the present work we investigate the residual resistivity induced by 3d atoms adatoms on Al in the framework of the Density Functional Theory in the Local Spin Density Approximation. Especially we focus on elucidating new features that are absent in the case of bulk impurities such as the dependence of the induced resistivity on the adatom position d from the surface. Some of such adatoms should also display a magnetic behavior, owing to the low density of the electronic surface tail, which may be absent in bulk. We adopt semi-infinite jellium to simulate an Al-like substrate and the problem is handled with the use of the embedding method of Inglesfield. Because of a spin polarization of some of the 3d adatoms, we found that the characteristic bell shaped curve of the induced resistivity as function of the atomic number Z is substituted by a double bell-shaped curve. Our results show that for some of 3d elements, the calculated induced surface resistivity as a function of d attains a maximum before decaying exponentially when the adatom is far away from the surface. In particular for Fe this occurs when this adatom is located at the chemisorption equilibrium position on clean Al. Detailed analyses of the induced density of states at the Fermi level indicate that such a maximum is explained in terms of the behavior of the adatom-induced DOS at the Fermi level.

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MULTICHANNEL ELECTRONIC TRANSPORT THROUGH A KONDO DOT

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Recent measurements of the electronic transport through a quantum dot (QD) of a nano-size showed [1] variety of phenomena. In the regime of weak coupling of the QD to electrodes the Coulomb blockade effects and the Kondo resonance for a medium range coupling were observed. A further increase of a tunneling rate leads to the conductance with a dip, which is characteristic for a Fano resonance. A similar effect was seen in transport measurements by the STM on magnetic adatoms [2].

We would like to present modeling of such the device, which is based a multichannel electronic transport through the QD with many levels. The current is determined within the nonequilibrium Green function technique, in which all multiple scattering and interference processes are taken into account. Assuming strong interactions between electrons on the QD, we can use the slave-boson (SB) technique to describe the Kondo resonance. The results are compared with those obtained by the equation of motion approach.

Our special attention is focused on inference processes between traveling waves through different levels, which can be considered as coupled Kondo impurities. First, the conductance is determined for a low source-drain voltage. Applying the gate voltage to the QD one can shift energy levels and change the interference conditions. The effect is well seen in the conductance, which changes its character showing the Fano resonance as well. We have also performed studies of the differential conductance dI/dV as a function of the source-drain voltage. The dI/dV curve shows a peak, which arises from the Kondo resonance. However, changing the interference conditions one can change the shape of dI/dV and the peak is continuously transformed to the dip.

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Electron-hole trapping and self-trapping in polyethylene

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An electron-hole pair, either excited optically (exciton), or injected by external fields, represents an exceedingly strong perturbation in a wide gap insulator. That is particularly true if, as in the case of polyethylene and other saturated organic molecular systems, the solid is held together by weak van der Waals forces, and can thus rather easily distort. Even in the perfect crystalline material, the question whether an electron hole pair would freely propagate, or whether it might instead generate a local distortion and become self-trapped by that, is highly relevant. We studied by *ab-initio* molecular dynamics simulations the behavior of an electron-hole pair in crystalline PE, and found that the pair becomes indeed self-trapped, with a trapping energy of 0.38 eV. The self-trapping is realized by the spontaneous appearance of a local distortion of the polymeric chain, consisting in a pair of trans-gauche conformational defects, 3 C_2H_4 units apart. Between these two defects, the chain is rotated by 120 degrees, creating a narrow inter-chain pocket, in whose neighborhood the electron and the hole become bound. The electron binding is tight, quite similarly to the free electron self-trapping state discovered in previous calculations, but the hole is only loosely bound, consistent with the lack of self-trapping for free holes. True polyethylene systems of practical use are neither crystalline nor pure. To understand the fate of an electron-hole pair in that case, we studied its behavior in polyethylene with three common chemical defects, namely: a) a grafted carbonyl (C=O); b) an intra-chain vinyl double bond (C=C); c) a grafted carboxyl (COOH). Each of these cases was investigated by *ab-initio* simulation, and found to lead to a different result, namely we found in the three cases: a) e-h trapping, stable at the C=0 graft; b) e-h trapping at the intra-chain vinyl double bond, however followed by radiationless recombination; c) bond-breaking, with formation of a COOH radical.

Dynamics and friction in incommensurate systems

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We study the dynamics of an incommensurate chain sliding on a periodic lattice, modeled by the Frenkel Kontorova hamiltonian with initial kinetic energy, without damping and driving terms. We show that the onset of friction is due to a novel kind of dissipative parametric resonances, involving several resonant phonons which are driven by the (dissipationless) coupling of the center of mass motion to the phonons with wavevector related to the modulating potential.

Furthermore, we show that invariance properties of the Lagrangian of this model imply the existence of a generalized angular momentum which is an integral of motion if the system remains floating. We find that, during the dynamics, the non-linear couplings of our model cause parametric phonon excitations which lead to the appearance of Umklapp terms and to a sudden deviation of the generalized momentum from a constant value, signalling a dynamical transition from a floating to a pinned state.

We conjecture that this transition can be seen as the dynamical equivalent of the Aubry transition for the static Frenkel-Kontotova model.

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Energy gaps and valence-level ordering in the cubic Hg II-VI compounds

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The established view of the zinc-blende structured Hg-based II-VI systems beta-HgS, HgSe and HgTe is that they are semimetals with an exactly zero fundamental energy gap, due to their inverted band-structure. Here it is argued, using symmetry properties combined with density functional calculations, that this picture should be revised.

It is demonstrated that in general, an inverted band-structure does not necessarily lead to a zero fundamental energy gap for systems with zinc-blende symmetry. Specifically, beta-HgS is found to have at the same time an inverted band structure, and a small, slightly indirect, fundamental energy gap.

The debated ordering of the highest valence levels in these systems is also discussed, and a mechanism, which would provide new experimental information on the subject is suggested.

Soft vibrations and acoustic-optic mode couplings in ferroelectrics with large piezoelectric responses

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There is great interest in piezoelectric materials for contemporary and future applications such as wireless communications, imaging and sonar, that rely on the interplay between mechanical and electrical energies. Much of current research is focused on the ferroelectric solid solutions $Pb[(Mg_{1/3}Nb_{2/3})_{1-x},Ti_x]O_3$ and $Pb[(Zn_{1/3}Nb_{2/3})_{1-x},Ti_x]O_3$ known as PMN-PT and PZN-PT. Single crystals of PMN-PT and PZN-PT exhibit large electromechanical coupling factors and piezoelectric strains as large as 1.7\% have been reported.

In PMN-PT and PZN-PT one of the end members, either $Pb(Mg_{1/3}Nb_{2/3})\ O_3$ (PMN) or $Pb(Zn_{1/3}Nb_{2/3})O_3$ (PZN), is a relaxor ferroelectric with a diffuse phase transition. The other end member, $PbTiO_3$ (PT), has a conventional transition from a paraelectric cubic perovskite phase to a ferroelectric tetragonal phase. The ferroelectric phases of PMN-PT and PZN-PT can have either tetragonal or rhombohedral unit cells. The two phases are separated by morphotropic phase boundaries. Enhanced piezoelectric responses occur at compositions close to the MPB's.

We studied the links between the behavior of vibrational modes and the structural phase transition. Raman spectra of $Pb[(Mg_{1/3}Nb_{2/3})_{1-x},Ti_x]O_3$ and $Pb[(Zn_{1/3}Nb_{2/3})_{1-x},Ti_x]O_3$ solid solutions reveal transverse optic vibration modes that soften with x and display remarkable changes in lineshapes when the compositions approach boundaries that separate ferroelectric phases with tetragonal and rhombohedral unit cells. The spectral lineshapes suggest interactions between acoustic and optic vibrations that manifest strong coupling between macroscopic strain and internal strain. These results provide evidence that intrinsic microscopic mechanisms, such as softening of the lattice and coupling between macroscopic strain and internal strain, coexist with the nanoscale disorder characteristic of relaxor ferroelectrics to create giant piezoelectric responses in these materials[1,2].

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Semiconductor Material Recognition, Nucleation and Control via Peptide Interfacing

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Control of crystal structure, phase, orientation and nanostructural regularity of inorganic materials is an ability uniquely seen in biological systems. We are currently investigating the principles of this natural biological molecular recognition in materials and developing new methods to pattern useful non-biological electronic materials on new length scales. Here we expedite biological selection through the use of genetically engineered viruses to find peptide recognition specific to interesting nanomaterials, such as zinc sulfide, cadmium sulfide, lead sulfide. These materials have unique optical, electrical and optoelectronic properties that can find potential technological applications and may lead to a wide variety of practical devices. This peptide combinatorial approach utilizes the inherent self-organizing, highly selective properties of biologically derived molecules. We have selected peptides that can nucleate and control aspect ratio and particle diameter of these materials. In aqueous, room temperature syntheses, these peptides show control over crystallographic structure and orientation of nanoparticles and nanowires. In addition, synthetic peptides and further genetic engineering techniques are being utilized to further show controlled nanoparticle crystal growth and arrangement. Using this peptide-directed recognition, we are organizing organic/inorganic materials into heterostructured assemblies.

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Observations of Coulomb Correlations in Elementary Excitations of the Ultra-Low Density 2D Electron Gas

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Studies of ultra-low density two-dimensional electron gases in semiconductor quantum structures are at current frontiers of condensed matter physics and materials science. Ultra-low electron densities with large carrier mobility can only be achieved in superior materials and thus demonstrate significant breakthroughs in fabrication methods. In our work we characterize such systems in GaAs/AlGaAs quantum structures and take advantage of the achievement of ultra-low density 2D electron gases to explore novel states of matter that arise from fundamental electron interactions. These studies cover a broad range of phenomena that include quantum Hall states [1-3], electron solids [4,5], and density-wave states [6,7].

We introduce resonant inelastic light scattering methods that have the sensitivity to identify collective excitations of ultra-low density 2D electron systems. In these studies we are able cover a broad range of interaction strengths. Through examination of collective excitation modes, we discovered that interactions play a significant role in the physics of the electron system well before they are large enough to cause a phase transition. Included in this presentation are recent results that demonstrate a high quality system with a density $n<8\times10^{8}\mathrm{cm}^{-2}$. These record low densities, which are lower than any previously published for a 2D electron gas in a semiconductor quantum structure, represent a current frontier in the field. This brings us tantalizingly close to the predicted electron solid regime [4], which should be readily distinguishable from gas or liquid phases in our inelastic light scattering experiments that probe wavevectors in the range of Fermi wavevectors.

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QUANTIZED PHONON SPECTRUM OF SINGLE-WALLED CARBON NANOTUBES

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A direct consequence of the cylindrical geometry of carbon nanotubes is that both the electronic and vibrational (phonon) states should be quantized in the circumferential direction. For the phonons, this should result in a one-dimensional phonon density of states that increases stepwise with increasing energy and displays sharp van Hove singularities at the step edges. We have probed the phonon energy spectrum of bundles of single-walled carbon nanotubes by measuring both their temperature-dependent specific heat[1] and their temperature-dependent thermal conductivity[2,3]. The specific heat data provide direct evidence of 1D quantization, and in addition probe the mechanical coupling between neighboring tubes in SWNT ropes. The measured specific heat is consistent with a tube-tube coupling that is much weaker than would be expected from simple comparison to graphite. This weak coupling has implications for both the mechanical and thermal properties of SWNT bundles. The thermal conductivity K(T) is consistent with 1D behavior, and preliminary results of measurements of K(T) using samples with varying average tube radius further support this picture.

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Berthelot - Type Anomalous Temperature Dependence And Quantum Confinement Model For Photoluminescence

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Abstract

Berthelot - type anomalous temperature dependence has been explained quantitatively and qualitatively. Relations between Berthelot-type temperature, maximum quantum confinement energy and effective exponent of size as a function of relative change of disorder and mean size. Calculations have been done for the internal quantum efficiency in terms of hopping and radiative rates. The fitting procedures between energy upshift and size have been used to understand the mechanism of photoluminescence and its spectra using quantum confinement model.

Mechanism for Appearance of Photonic Band Gap and Infiltrated Synthetic Opal as Photonic Crystal

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Abstract

The mechanism of threshold effective refractive index in addition to that of density of states minimum is proposed within optimum scattering strength for silicon as background material and air as dielectric. The optimum scattering strength is 1.61 and minimum effective refractive index is 1.38 at 92% volume filling fraction for air atom. Calculated values of relative width and lattice size for nematic liquid crystal ZLI-1132 and smectic liquid crystal (R)-4'-(1-mathoxycarbonyl-ethoxy)-phenyl-4-[4(n-octyloxy)phenyl] benzoate (1MC1EPOPB) synthetic opal ($Si0_2$) infiltrated with liquid crystal as a function of temperature using a model of strong localization for the occurrence of pseudogap are reported.

Tunneling Between Two-Dimensional Electron and Hole Gases

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We have calculated the tunneling current between a two-dimensional (2D) electron gas and 2D hole gas separated by a potential barrier, as a function of the voltage difference between the two gases. Our calculation takes into account energy and parallel-momentum conservation and many-body effects through the spectral distribution function. We have found that, unlike the case of tunneling between 2D electron gases, the current is non-zero for a broad voltage range. A comparison with I-V characteristics of InAs/AlSb/GaSb/AlSb/InAs heterostructures, in which 2D electrons and holes accumulate in the InAs and GaSb regions, respectively, yields a qualitative agreement between theory and experiment. A quantitative comparison may require the inclusion in the calculations of effects such as electron-electron, electron-hole, and electron-phonon interactions.

Reference: Phys. Rev. B 63, #033308 (2001)

Quantum Annealing of the Two Dimensional Ising Spin Glass

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Recent experiments by the NEC group [1] on Li Ho_x Y_(1-x) F_4 -- a disordered Ising ferromagnets -- have shown that annealing obtained through the application of a transverse magnetic field appears to be much more effective then a standard thermal annealing.
Motivated by these experiments we started a theoretical study of the short range Ising spin glass models in two dimensions using both thermal annealing (through standard classical Monte Carlo) and quantum annealing, attained by introducing a decreasing transverse (spin-flip) field term in the Ising Hamiltonian. Quantum annealing is performed by means of Path Integral Monte Carlo and Green function Monte Carlo techniques.

In order to characterize and compare the efficiency of the two different annealing methods, we studied the dependence of the residual energy, i.e. the energy attained after sending either temperature or transverse field to zero, upon the cooling rate $1/\tau$. In the classical/quantum annealing procedure, τ is identified with the (Monte-Carlo) time at which the temperature/field, initially finite, have been linearly decreased to zero.
We looked at the residual energy obtained by repeteadly annealing single realizations of the disordered couplings for 32x32, 48x48, and 80x80 lattices. For each of those realizations, the exact ground state was calculated exactly using the Koeln spin-glass server [2]. Our Monte Carlo simulation results for those cases suggest that both thermal and quantum annealing give a residual energy that converges to the exact ground state with a behavior consistent with the Huse and Fisher theory [3], i.e. (1/log τ)^β. However, the exponent β appears to be larger for the quantum annealing.

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Towards extending the applicability of density functional theory to weakly bound systems

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Abstract

While the attempts currently in progress in several groups for the rigorous inclusion of dispersion interactions in Density Functional Theory (DFT) calculations mature and evolve into practical methodology, we contribute to the debate on the applicability of current functionals to the calculation of weak interaction with a systematic investigation of a few, typical, weakly bound systems. We have used both pure DFT and a hybrid approach in which the total interaction energy is partitioned into two parts: a) the dispersion energy which, in a first approximation is the contribution due to intermonomer correlations and b) all other interactions. The first component is accurately obtained at all *distances of interest* by means of the well known *damped* multipolar expansion of the dispersion energy while for the second component different approximation will be evaluated. The need to avoid double counting a fraction of the correlation energy when using the hybrid approach and the choice of the appropriate functionals are also discussed. We consider four systems of increasing binding strength, namely the Ar_2 and Kr_2 dimers, the benzene dimer, the water dimer, and a few metal carbonyls. For pure DFT calculations we confirm the conclusion reached by others concerning a) the strong dependence of the results on the choice of the functional for dispersion-dominated interaction (noble gases and benzene) with the overall tendency to yield underbinding and b) the relatively accurate, functional-independent, description of that DFT gives of water, which we attribute to the fact that this system is dominated by electrostatic interactions. For the carbonyls we find that DFT yields results which are again strongly dependent on the choice of the functional and show a tendency to give overbinding. Our hybrid method shows instead shortcomings only for the noble gases. The problem in this case is traceable to the well-known difficulties that all current functionals experience at medium-large intermonomer separations. The quality of the hybrid results improves markedly for benzene due to the large value of both dispersion and repulsive interactions at the equilibrium distance for this dimer, which makes the balance between the two, less delicate. Excellent results are also obtained for water (for the same reason as indicated above) and more significantly for the carbonyls where we find that dispersion contributes to the binding more than it could be guessed *a priori*. We do not claim to have found a general solution to this difficult problem, but we aim at providing a quantitative assessment of where the problems are pointing at directions from which a general solution may, eventually, emerge.

Chiral Current in Helical Nanowires

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Very recently, the gold nanowires were formed in gold thin films by electron-beam irradiation in an ultrahigh vacuum. Transmission electron microscopy images showed that they take helical configurations [1]. Prior to the experimental observation, using empirical molecular dynamics, it was predicted that even for metals with isotropic atomic potentials, the helical structures could be stable when the diameters are smaller than the critical values [2]. More recent theoretical investigation revealed that the helical structures are stabilized as a result of optimization of surface and interior (bulk) energies [3]. It is well recognized that the conductivity of carbon nanotubes changes drastically from metallic to semiconducting/insulating depending on the chirality of a tube. On the other hand, the conductance of the helical gold nanowires has not been measured yet. Therefore it is an interesting problem to clarify whether the similar conductance changes take place in metallic nanowires with helical configurations. Moreover, it is also very interesting to clarify whether chiral current can be observed or not. In the present study, we investigated such subjects numerically (using recursion-transfer-matrix method) as well as analytically.

We adopted the jellium model where electrons are confined in a uniform potential with boundary of the helical geometry. The shapes of cross sections were approximated by regular polygons, having N-fold symmetry.

As a result, we found that there appear characteristic humps and dips with steps of $1G_0$ or $2G_0$ $(G_O = 2e^2/h)$ in conductance curves as a function of electron energy, when L_H (the pitch of the helix) is in a certain range. The anomalous conductance was revealed analytically to originate from the fact that an energy gap opens due to noncircular cross section and shifts toward higher energies with decreasing L_H [4]. We also found that the chiral current flows only at energies where the energy gap appear. This means that the chiral current can not be observed if the electron energy is outside of such an energy gap region even though the nanowire is helical.

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Manipulating Spin Coherence in Semiconductor Nanostructures

Martino Poggio

Coherently controlling electron and nuclear spins in semiconductor
nanostructures provides a promising means of manipulating and storing quantum information. Since optically injected spin-polarized electrons can be used to polarize, detect, and manipulate nuclear spins (1), it is important to understand the mechanisms responsible for electron spin decoherence in the solid state. To this end, time-resolved Faraday rotation spectroscopy is used to measure spin coherence in systems with dramatically different structural integrity: n-type GaN epilayers and n-type GaAs (2).
Spin coherence in GaN epilayers with densities of charged threading
dislocations of 5*10^8 cm^-2 yields lifetimes of ~20ns at T=5K and persists to room temperature. Although momentum scattering is strongly enhanced by these defects, spin coherence appears surprisingly robust. Despite the presence of several orders of magnitude greater defect densities in GaN, the dynamics of electron spins are qualitatively similar to the dynamics in the more ordered GaAs systems, suggesting a common origin for spin relaxation.
Such relaxation mechanisms include the hyperfine coupling to nuclei, which can be controlled to perform NMR in nanostructures (3).

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Melting properties of an alkali halide (100) surface

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Abstract

Molecular dynamics simulations based on the Fumi-Tosi potential are used to study the melting habit of NaCl, and of the NaCl (100) crystal surface.

We find first of all a gratifyingly realistic description of bulk thermal expansion, of bulk melting (T_m = 1142 K calculated against 1070 K experimental), and of the volume increase at melting (25.16% calculated at zero pressure against 26.08% experimental).

The NaCl (100) surface is found to remain solid up to and above the bulk melting temperature, seemingly a classic case of surface non-melting. Accordingly, we find it possible to overheat the surface up to 200 K above the bulk melting point. Our results show also the possibility of a surface freezing.

Conduction Channel Blocking and Magnetization Reversal in Nickel Nanowires

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Experimental data have recently appeared indicating that the lowest conductance step for a Ni tip touching a Ni substrate can be, at least in presence of a magnetic field, fractional, and quite close to one half of the conductance quantum [1].
We have carried out electronic structure calculations for an extremely idealized Ni nanobridge consisting just of monatomic nanowire, which show that under certain circumstances the d-state ballistic conductance channel may be blocked, but the s-p channel not. Within our density functional approximation, blocking is connected with magnetism, specifically with a reversal of magnetization direction localized at the idealized atomic point contact. The next question concerns the role of the external magnetic field, since under experimental conditions a long-range magnetization is probably present anyway both in the Ni tip and in the Ni substrate. Preliminary calculations indicate that while a magnetically symmetric configuration will still have both up and down spin open channels and thus integer conductance, introduction of a small magneticasymmetry about the idealized contact point seems capable of eliminating one of the spin channels, reducing conductance in the s-p channel from two to one.

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Effect of crystal bending on surface melting

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Surface melting, well established and documented for many metals and nonmetals, is generally a delicate phenomenon to characterize experimentally. The reason is that the thickness of the liquid film present in equilibrium above the solid surface is microscopically small, at most a few monolayers even a fraction of a degree below the bulk melting point.

In this respect, the availability of an external non-thermal tool capable of enhancing, or anyway of controlling and modifying the equilibrium liquid layer thickness would be of great value.

We propose here that surface strain exerted on the crystal for example though bending, can constitute such a tool. The idea is that elastic energy stored in the strained crystal surface can be released once the surface melts. Therefore we expect that a bent solid slab should show enhanced surface melting, resulting in an increased liquid layer thickness relative to the strain-free solid, on *both* faces, the "stretched" as well as the "compressed" one.

To test this idea, we are conducting extensive molecular dynamics simulations for the Al(110) surface, where surface melting is well documented [1,2,3,4]. The slab geometry permits a direct comparison of negative and positive strains on the two faces. Availability of the Ercolessi-Adams potential for Al makes this study particularly realistic, so that the results obtained in these simulations should be immediately comparable with experiments, that are not yet available.

Preliminary results indicate that bending-enhanced surface melting should indeed take place close to the melting temperature. The typical magnitude of the effect will be compared with simple estimates based on surface thermodynamics. We also plan to investigate whether the detailed behavior of the two faces, concave and the convex, will as we expect display some microscopic differences.

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THE NONLINEAR THERMOMAGNETIC DISSIPATIVE STRUCTURES IN HIGH TEMPERATURE SUPERCONDUCTORS

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Abstract

At present, superconducting magnetic systems high critical field strengths and current densities are widely implemented introduced in different areas of modern science and technology. However, successful operation of the superconducting materials is only possible provided that special measures are taken to prevent a system from the thermal or magnetic breakage of superconductivity and the transition to a resistant state. For this reason, one of the main problems in the investigation of properties of superconductors is that predicting the superconducting state breakage caused by dissipative and nonlinear effects related to viscous motions of the magnetic flux. This explains a considerable interest in the study of dissipative and nonlinear effects in superconductors that has arose in recent years [1].

Linear stage of unstability is studied sufficiently. It is necessary to take into account dissipative and dispersion factors connected with Joule heat in superconducting state during the study of evolution dynamics thermomagnetic unstability in the framework of nonlinear approach. In such situations under determined conditions unstability leads to selforganization, i.e. to emerging the stabile and stationary nonlinear dissipative structures of type of the shock wave or soliton observed by us in superconductors in early studies [2].
Mechanisms of origin and dynamics of development of nonlinear stationary thermomagnetic waves, as well as their structure and velocity of propagating, stability comparatively to small fluctuations we have studied sufficiently.

In this work to analysis of the nonlinear dynamics of thermal and electromagnetic perturbations in superconductor caused by dissipative effects involved in the viscous motion of the magnetic flux is studied.
The structure and evolution of the stationary thermomagnetic waves propagating in the superconductor is studied based on a system of nonlinear equations describing dynamics of the instability development in the system studied. The appearance of these structures is qualitatively described and the wave propagation velocity is estimated.

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