Report

Theoretical Modeling of Transport in Nanostructures
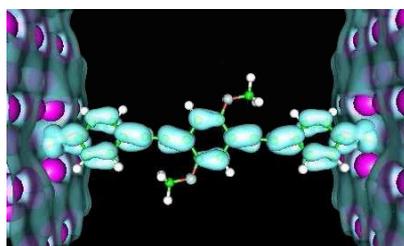
Dates :
Jun 02, 2009 - Jun 05, 2009

Location :
CECAM-HQ-EPFL, Lausanne, Switzerland

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1 Details

1.1 Description

Start: 2 June 14.30
End: 5 June 12.30

Interest in electronic transport properties of molecular wires and junctions has continuously increased during the last decades. The basis for this interest comes both from a fundamental scientific viewpoint and the possibility of technological applications as current electronic devices continue to shrink. Recently, for example, European researchers have measured the conductance of (i) a single hydrogen molecule [1], (ii) gold wires up to seven gold atoms long [2], and (iii) more complex hydrocarbon molecules [3,4]. The modelling of transport properties in (i) the phase coherent regime and (ii) Coulomb blockade regime has made similar strides where several European groups have independently developed atomistic computational methods to deal with the theoretically difficult non-equilibrium and finite-dimensional transport problem [5,6,7,8,9,10]. Especially methods using density functional theory to model phase coherent transport have been extended to include inelastic effects, spin polarized currents, and non-collinear magnetization.

Despite the fact that many of the developments in modelling were archived by research groups in Europe, the lack of workshops/conferences hinder the dissemination and discussion of resent results. The main purpose of the suggested workshop is thus to increase the interactions between the researchers working on computational modelling of transport properties. In addition, many new developments including the modelling of spin polarized transport, inelastic scattering (phonon, magnon, photon), and thermoelectric properties (interaction of heat and electrical transport) are of interest.

Current ab-initio methods based on density functional theory (DFT) allow the calculation of the transport properties of systems with hundreds of atoms [5,6,7,8,9,10], both at zero bias and under the presence of a finite voltage. These systems include molecules between metallic or semiconducting leads, atomic constrictions and chains, nanowires and nanotubes. In general, the transport properties of molecules strongly bound to the electrodes agree qualitatively but not quantitatively with experiments, with both the low-bias gap and absolute value of the current being too large [11]. However, the agreement is getting better as the codes and theory improve and excluding a few cases (like the archetypical Au-BDT junction [12]) the differences between theory and experiment are within one order of magnitude [13]. Several attempts have been made to increase the applicability of DFT methods, to include inelastic effects, spin degrees of freedom, non-collinear magnetism, the spin-orbit interaction, and beyond-DFT approaches like self-interaction effects, GW approaches, and time-dependent DFT (TDDFT). The aim at present is to develop feasible approaches to determine more accurately the transport properties of a wide range of molecules.

2 Program

Day 1 - June, 2nd 2009

- 14:30 to 15:00 - Welcome
- 15:00 to 15:30 - **Colin Lambert**
  Controlled Electron Transport Through Single Molecules
- 15:30 to 16:00 - **Harold Baranger**
  Strong Correlations in Quantum Dots and Wires: Quantum Monte Carlo Studies
- 16:00 to 16:30 - **Victor Geskin**
  Partial vs. integer electron transfer in molecular assemblies: on the importance of multideterminant theoretical description and the necessity to find a solution within DFT
- 16:30 to 17:00 - Coffee Break
- 17:00 to 17:30 - **Mike Ford**
  Density Functional based calculations for nanostructures containing large numbers of atoms
- 17:30 to 18:00 - **Supriyo Datta**
  Nanodevices and Maxwell's Demon

Day 2 - June, 3rd 2009

- 09:00 to 09:30 - **Kurt Stokbro**
  New developments for ab initio and semi-empirical modeling of quantum transport in electronic devices
- 09:30 to 10:00 - **Michael Galperin**
  Optical response of current-carrying molecular junctions
- 10:00 to 10:30 - **Tomasz Kostyrko**
  A quest for a molecular diode based on the mechanism of elastic scattering in asymmetric junctions
- 10:30 to 11:00 - Coffee Break
- 11:00 to 11:30 - **George Kirczenow**
  Theoretical Modeling of Transport in Molecular Nanostructures: A Pragmatic Approach
- 11:30 to 12:00 - **Frederico Novaes**
  Tunneling across a ferroelectric barrier: a first-principles study
- 12:00 to 12:30 - **Fabian Pauly**
  Controlling transport properties by molecular structure and light
- 12:30 to 15:00 - Lunch Break
- 15:00 to 15:30 - **Ferdinand Evers**
  Interplay of charging, conformation and magnetisation in metal (II) organic

complexes: a DFT study
- 15:30 to 16:00 - **Juan José Palacios**
  Spintronics with graphene nanoribbons
- 16:00 to 16:30 - **Ivan Rungger**
  Bound and weakly coupled states in electron transport calculations
- 16:30 to 17:00 - Coffee Break
- 17:00 to 17:30 - **Anna Delin**
  Nanomagnetic phenomena in transition metal nanowires
- 17:30 to 18:00 - **Tchavdar Todorov**
  Can current drive an atomic-scale motor?
- 18:00 to 19:30 - Poster Session

Day 3 - June, 4th 2009

- 09:00 to 09:30 - **Daniel Sanchez Portal**
  Tilt angle dependence of electronic transport in molecular junctions of self-assembled alkanethiols
- 09:30 to 10:00 - **Alessandro Pecchia**
  NON-EQUILIBRIUM GREEN's FUNCTIONS AND DENSITY FUNCTIONAL TIGHT-BINDING: A CRITICAL REVIEW AND PERSPECTIVES OF FUTURE DEVELOPMENT
- 10:00 to 10:30 - **Kristian Thygesen**
  Incorporating Exchange-Correlation Effects in Quantum Transport through Nano-scale Junctions
- 10:30 to 11:00 - Coffee Break
- 11:00 to 11:30 - **Robert Stadler**
  Interference effects and Fermi level alignment in electron transport through nitro-benzene nano-junctions
- 11:30 to 12:00 - **Alessandro Troisi**
  Microscopic Modelling of charge transport in molecular crystals, polymers and liquid crystals
- 12:00 to 12:30 - **Thomas Frederiksen**
  Electron-vibration couplings in single-molecule junctions
- 12:30 to 12:45 - **Kurt Stokbro**
  Software demonstration from QuantumWise A/S
- 12:45 to 15:00 - Lunch Break
- 15:00 to 15:30 - **Peter Bokes**
  Stroboscopic wavepacket basis for time-dependent quantum transport simulations
- 15:30 to 16:00 - **Alexandre Reily Rocha**
  Electronic transport in disordered systems: from gas sensors to spintronics
- 16:00 to 16:40 - **Pablo Ordejon**
  Transport in graphene layers connected by carbon nanotubes
- 16:30 to 17:00 - Coffee Break
- 17:00 to 17:30 - **Kyungwha Park**
  First-principles study of electron transport through the single-molecule magnet Mn12

- 17:30 to 18:00 - **Carl-Olof Almbladh**
  Kadanoff-Baym dynamics in strongly correlated nanostructures
- 20:00 to 23:00 - Dinner

Day 4 - June, 5th 2009

- 09:00 to 09:30 - **Andrés Arnau**
  Generalization of Bardeen's transfer Hamiltonian method to include inelastic currents due to electron vibration coupling
- 09:30 to 10:00 - **Jing-Tao Lu**
  Atomic dynamics in the presence of electronic current: Semi-classical Langevin equation approach
- 10:00 to 10:30 - **Stephan Roche**
  Computational Strategies to Tackle Mesoscopic Transport & Device Simulation in Complex Low-Dimensional Structures
- 10:30 to 11:00 - Coffee Break
- 11:00 to 11:30 - **Alexander Smogunov**
  Electron transport across locally magnetic nanocontacts
- 11:30 to 12:00 - **Zeila Zanolli**
  Defective carbon nanotubes: magnetism, spin transport and gas sensing applications
- 12:00 to 12:30 - **Mads Engelund**
  Heat Transport and Localized Vibrational Modes in Mono-Atomic Gold Chains
- 12:30 to 12:40 - Closing word

3 Participant List

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4 Abstract list

Computational Strategies to Tackle Mesoscopic Transport & Device Simulation in Complex Low-Dimensional Structures

Stephan Roche
CEA, Institut of Nanosciences and Cryogenics (FRANCE) and TU-Dresden (Germany)

Abstract

In this talk, I will discuss several quantum transport phenomena in chemically-modified forms of carbon nanotubes and graphene based materials and devices [1]. Several computational strategies (Kubo, Landauer-Buttiker, tight-binding or fully ab-initio) will be shown to allow realistic transport simulation, allowing in particular the extraction of transport length scales such as elastic mean free path and localization lengths, and to envision realistic nanoscale device simulation.

To start with, mesoscopic transport in chemically-doped or functionalized carbon nanotubes will be discussed, with for the
first time a complete study of the transition from weak to strong localization regimes in realistic models of low dimensional disordered systems [2]. In particular, the fundamental Thouless relationship will be shown to be well reproduced, demonstrating the robustness and predictability efficiency of the approaches.

In a second part, transport properties of 2D disordered graphene
will be analyzed in the case of short range disorder. In agreement with the conventional 2D localization scaling theory, the system will be shown to undergo a conventional 2D Anderson transition in the low temperature limit. The sensitivity of localization phenomena in regards to edge symmetries and change of transport dimensionality will be further outlined [3], and finally, the effect of more realistic chemical disorder on in 2D graphene transport will be analyzed [4].

Key References

[1] J.C. Charlier, X. Blase and S. Roche, Rev. Mod. Phys. 79, 677 (2007). A Cresti et al., Nano Research 1, 361-394 (2008).

[2] R. Avriller, S. Latil, F. Triozon, X. Blase, S. Roche, Phys. Rev. B 74, 121406R (2006); ibidem Modern Physics Letters B 21, 1955 (2007). A. Lopez-Bezanilla et al. Nano Letters 9 (3), 940 (2009).

[3] A. Lherbier, B. Biel, Y.M. Niquet, S. Roche, Phys. Rev Lett. 100, 036803 (2008). A. Lherbier, X. Blase, Y.M. Niquet, S. Roche, Phys. Rev Lett. 101, 036808 (2008).

[4] B. Biel, X. Blase, F. Triozon, S. Roche, Phys. Rev. Lett 102, 096803 (2009). B. Biel, F. Triozon, X. Blase, S. Roche (submitted).

Optical response of current-carrying molecular junctions

Michael Galperin
University of California at San Diego
Coauthor(s) : Abraham Nitzan and Mark A. Ratner

Abstract

Recently optical properties of biased molecular junctions started
to attract attention of researchers. Optical response (in particular Raman scattering) measurements together with the conductance of single molecule junctions promises to become a superior diagnostic tool. Theoretical understanding of optical response of biased junctions is of major importance for development of molecular optoelectronic devices. We discuss optical response of current-carrying molecular junction within a simple 2-level (HOMO-LUMO) model. Besides coupling to the contacts and molecular vibration, the model takes into account interaction with external (radiation) field and electron-hole excitations in the contacts. We use the approach to study absorption, fluorescence, and Raman spectroscopy of such junctions, as well as possibility of light and excitation induced currents.

Key References

M.Galperin, M.A.Ratner, and A.Nitzan. Nano Lett. ASAP (2008).
M.Galperin, M.A.Ratner, and A.NItzan. J. Chem. Phys. (submitted).
M.Galperin and A.Nitzan. Phys. Rev. Lett. 95, 206802 (2005).
M.Galperin and A.NItzan. J. Chem. Phys. 124, 234709 (2006).
M.Galperin, A.Nitzan, and M.A.Ratner. Phys. Rev. Lett. 96, 166803 (2006).

New developments for ab initio and semi-empirical modeling of quantum transport in electronic devices
Kurt Stokbro
University of Copenhagen, Denmark

Abstract

In this talk I will present the general framework of non-equilibrium quantum transport calculations[1] and present new algorithms[2,3] that reduce the computational time of the calculations by an order of magnitude and thereby strongly increasing the size of systems which can be addressed. Application of the model to various carbon systems will be presented.
The reduction in the computational time is obtained by both reducing the time for calculating the electrode selfenergy by using an iterative scheme utilizing a reduced Krylov space[2] and a new parallel algorithm for the Greens function calculation[3]. With this approach it is possible to simulate quantum systems with several thousand atoms. In order to include the effect of external gate electrodes we incorporate a multigrid Poisson solver which allow for defining continuum regions with fixed electro-static potential or dielectric constant.
The scheme has been implemented in a Semi-empirical Huckel Tight-Binding model, and the model has been applied to model a Carbon NanoTube with a triple gate. Result of the simulation will be presented and compared with experimental results.

The figure shows the self-consistent electrostatic potential at the atomic positions of a (4,2) carbon nanotube upon application of gate potentials of (-2,0,-2) (blue curve) and (-2,5,-2) (red curve).

Key References

1. K. Stokbro First Principles modeling of electron transport, J. of Physics Cond. Mat. 20, 064216 (2008).
2. H. H. B. Sørensen, P.C. Hansen, D.E.Petersen, S. Skelboe and K. Stokbro, Efficient wave function matching approach for quantum transport calculations, preprint http://xxx.lanl.gov/abs/0804.4306
3. D. E. Petersen et. al., A hybrid method for the parallel computation of Green's functions, Preprint.

Electronic transport in disordered systems: from gas sensors to spintronics

Alexandre Reily Rocha
Universidade Federal do ABC, Brazil
Coauthor(s) : Adalberto Fazzio and Antônio José Roque da Silva

First-principles study of electron transport through the single-molecule magnet Mn12

Kyungwha Park
Virginia Tech

Abstract

Recently, there have been significant experimental efforts to build and characterize single-molecule magnets bridged between electrodes, as well as theoretical efforts to study the systems based on model Hamiltonians. Single-molecule magnets showed various quantum effects including magnetic quantum tunneling and quantum interference. There is still a lack of understanding on
the effect of local environments on the electron transport
through single-molecule magnets. We examine electron transport through the single molecule magnet Mn12 using the non-equilibrium Green's function method in conjunction with density-functional theory. Considering two molecular geometries attached to Au electrodes, we discuss the coupling between the Mn12 and the electrodes as well as the charge distribution of conduction electrons over the Mn12 depending on different molecular geometries and interfaces. We also present a possibility of the Mn12 being used as a spin filter at low bias voltages.

Tunneling across a ferroelectric barrier: a first-principles study

Frederico Novaes
ICMAB-CSIC, Barcelona, Spain
Coauthor(s) : D. Bilc ,P. Ordejon ,J. Iniguez ,P. Ghosez

Abstract

Ferroelectric tunnel junctions (FTJ), including a ferroelectric as the barrier material, have recently attracted a lot of interest since they are potentially interesting for technological applications such as data storage. In such system, the barrier has to be sufficiently thin to allow for tunneling but must at the same time remain ferroelectric, a property that tends to be suppressed in ultrathin films. Up to now, the modeling of FTJ has remained at the semi-empirical level. Here, we consider a prototypical system made of a ferroelectric oxide film between two gold electrodes and compute the I-V curve of the system using density functional theory and Non-Equilibrium Green's Function (NEGF+DFT) formalism. Our atomic-scale approach allows for the first time accurate and self-consistent description of the screening at the metal ferroelectric interface and of the atomic relaxation. It predicts that the asymmetry in the I-V curve for up and down polarizations is sufficiently large to be detected experimentally, therefore opening the door to applications in which the tunneling current allows the reading of the polarization state. Work supported by FAME-EMMI.

Controlled Electron Transport Through Single Molecules

Colin Lambert

School of Physics and Materials, Lancaster University

Abstract

Measurement of the electrical properties of single molecules has only recently become an experimental reality. In this talk I shall discuss a range of geometrical methods for controlling electron transport through single molecules, including:

• ring rotations in conjugated molecules;
• Fano resonances associated with side groups attached to rigid backbones;
• solvation shells of analyte molecules in the vicinity of a conducting backbone;
• varying the angle of contact to conducting electrodes
• rotating the magnetic moments of carbon-nanotube-encapsulated molecules.

As well as the control of electrical currents via geometry, the inverse effect is discussed, whereby the geometry of a nanoscale conductor is controlled an electrical current. This is exemplified by carbon-nanotube windmills, whereby an electrical current causes an inner chiral tube of a double-wall nanotube to rotate.

Key References

1. Precision control of single-molecule electrical junctions, W. Haiss, C. Wang, I. Grace, A. S. Batsanov, D. J. Schiffrin, S. J. Higgins, M. R. Bryce, C. J. Lambert and R. J. Nichols, Nature Materials 2006, 5, 995.
2. Towards molecular spintronics, A. Reily Rocha, V. M. García-Suárez, S. W. Bailey, C. J. Lambert, J. Ferrer and S. Sanvito, , Nature Materials 2005, 4, 335.
3. Tuning the electrical conductivity of nanotube-encapsulated metallocene wires, V. M. García-Suárez, J. Ferrer and C. J. Lambert, Phys. Rev. Lett. 2006, 96, 106804.
4. Control of electron transport through Fano resonances in molecular wires, T.A. Papadopoulos, I.M. Grace and C.J. Lambert, Phys. Rev. B74 193306 (2006)
5. Carbon nanotube electron windmills: A novel design for nanomotors
S.W.D. Bailey, I. Amanatidis, and C.J. Lambert, Phys. Rev. Lett. 100, 256802 (2008)

Partial vs. integer electron transfer in molecular assemblies: on the importance of multideterminant theoretical description and the necessity to find a solution within DFT

Victor Geskin

Université de Mons-Hainaut

Coauthor(s) : Robert Stadler, Jérôme Cornil

Stroboscopic wavepacket basis for time-dependent quantum transport simulations

Peter Bokes

Slovak University of Technology

Abstract

Time-dependence in quantum transport is a complex issue. On the one hand, it gives us the non-equilibrium steady-state upon switching-on of the bias voltage and thereby helps to identify the correct stationary density matrix, or it facilitates a description of rapid time-dependent processes combined with transport. On the other hand, it raises many new questions regarding the importance of particular form of

the switching-on, importance of interactions with a bath or reservoir or the correct description of exchange and correlation effects in transport. I will demonstrate that many of these questions can be addressed with a surprising clarity using a novel stroboscopic wavepacket basis sets [1]. These represent basis sets specifically tailored for a description of time-dependent processes in extended systems like non-periodic geometries of various contacts consisting of solids and molecules. In my talk I will explain properties and construction of such a basis for simple finite systems but most importantly for general extended systems with continuous spectrum. Introducing of the interaction representation one can take the full advantage of the time-dynamics built into the basis and hence simulate infinite open systems without the need of the more conventional tool - the leads' self-energies. The formalism will be demonstrated on a semi-analytical example of electronic transport through resonant tunneling barrier in 1D [2] where it gives a simple elucidation of various time-scales in the process of switching on the bias. In the second example the wavepacket basis will be used to study scattering of electrons on localised phonon mode in a simple lattice model.

Key References

[1] P. Bokes, F. Corsetti, R. W. Godby, Phys. Rev. Lett. 101, 046402 (2008)
[2] P. Bokes, cond-mat/0902.1600, accepted in PCCP (2009).

Can current drive an atomic-scale motor?

Tchavdar Todorov
Queen's University Belfast
Coauthor(s) : Daniel Dundas, Eunan McEniry

Abstract

This question hinges on the problem of whether or not current-induced forces on atoms are conservative: they must be non-conservative, to enable net work to be done, on a suitable rotor, per revolution. This talk will give a short discussion of past arguments for and against conservatism. It will then be shown analytically that forces on atoms under steady-state current in a nanowire are not conservative, and that this makes it possible, in principle, for current to drive individual atoms around, like waterwheels. Some of the factors that could control - and limit - the practical feasibility of such an atomic-scale motor will be discussed at the end.

Theoretical Modeling of Transport in Molecular Nanostructures: A Pragmatic Approach

George Kirczenow
Simon Fraser University, Canada

Abstract

Modeling electrical conduction through individual molecules or small groups of molecules presents significant challenges. These include the lack of detailed knowledge of the atomic geometries of the experimental systems and the presence in many cases of a complex and not fully characterized environment surrounding the molecule such as an organic solvent or aqueous medium, an electrolyte and/or (often unknown) adsorbates on the electrode surfaces. Furthermore, the application of the standard ab initio time-independent density functional approximations such as the LDA, GGA and their relatives to transport in molecular junctions does not have a rigorous justification and is increasingly being questioned in the recent literature.

Given these difficulties, keeping the modeling simple (but not too simple) has significant advantages. Experience has shown that extended Huckel theory with a standard parameterization developed over the years by chemists to describe the quantum mechanics of many molecules, modified so as to also describe the electronic structures of crystal electrodes, supplemented where necessary by those aspects of density functional theory that are well justified, and by phenomenology where that is needed, can provide valuable insights into experimental observations and yield interesting predictions. In this talk I will discuss some examples of what can be learned using this pragmatic approach. Topics will include electrical conduction in molecular heterolines on silicon, single-molecule electron transport in oligopeptides and proteins, and single-molecule electroluminescence, time permitting.

Heat Transport and Localized Vibrational Modes in Mono-Atomic Gold Chains

Mads Engelund
DTU Nanotech
Coauthor(s) : Mads Brandbyge, Antti-Pekka Jauho

Abstract

We have developed an ab-initio method for evaluating the vibrational properties of a contact between two surfaces. In order to calculate the vibrational behaviour we perform density-functional theory (DFT) calculations to relax the structures and calculate the dynamical matrix using finite-difference DFT calculations. This method is used to investigate heat transport and damping of vibrational modes in mono-atomic gold chains of different lengths and states of strain. Our results show, in agreement with previous estimates [1], that the damping can be very low (Q-factors up to ~1500). However, we find that the damping rate can vary by more than an order of magnitude for a relatively small change in strain (0.03 Å elongation pr. bond in the chain). On the other hand, the heat conductance is found to be a relatively smooth function of strain. The magnitude of the heat conductance is comparable to the bulk conductance pr. surface unit cell for the low index directions.

Key References

[1]: Frederiksen et al., Phys. Rev. B 75, 205413(R)(2007)

Atomic dynamics in the presence of electronic current: Semi-classical Langevin equation approach

Jing-Tao Lu
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Coauthor(s) : Mads Brandbyge and Per Hedegård

Abstract

We derive and calculate the atom dynamics of a molecular junction in the presence of electrical current by a semi-classical Langevin equation. In this description the non-equilibrium electronic environment is described like an effective "bath" influencing the atomic dynamics [1]. The effective bath induces fluctuation (colored noise) and dissipation (friction force) on the atoms.

We identify new forces acting on the atoms due to the non-equilibrium in the bath. These include e.g. the "Joule heating", and the non-conserving force, recently discussed by Todorov and co-workers [2]. We first illustrate and analyze the consequences of these new effects using a minimum tight-binding model, and then do first-principles DFT calculations on atomic chain systems[3,4] in order to address the importance of the different non-equilibrium forces in realistic atomic-scale conductors.

References
[1] M. Brandbyge, P. Hedegård, Phys. Rev. Lett. 72, 2919 (1994).
[2] D. Dundas, E. J. McEniry, T. N. Todorov, Nature Nanotechnology 4, 99-102 (2009).
[3] M. Brandbyge et al., Phys. Rev. B 65, 165401 (2002)
[4] T. Frederiksen, M. Paulsson, M. Brandbyge, A.-P. Jauho, Phys. Rev. B 75, 205413 (2007).

Nanodevices and Maxwell's Demon
Supriyo Datta
Purdue University

Abstract

Maxwell invented his famous demon to illustrate the subtleties of thermodynamics and energy conversion, and his conjecture has inspired much discussion ever since. Technology has now reached a point where it is possible to build electronic Maxwell's demons that can be interposed between the two contacts (source and drain) of a nanoscale conductor (the channel) to allow electrons to flow preferentially in one direction so that a current flows in the external circuit even without any external source of energy. I will use this device to illustrate some of the subtleties of quantum transport that theoretical models need to capture.

Defective carbon nanotubes: magnetism, spin transport and gas sensing applications
Zeila Zanolli
Catholic University of Louvain, Louvain-la-Neuve
Coauthor(s) : Jean-Christophe Charlier

Abstract

Carbon nanotubes (CNTs) are renowed in the scientific community for being both a playground for studying fundamental physical properties and for applications in, to mention a few, electronic, spintronic and gas sensing technologies. However, despite the progresses in growth techniques, CNTs always exhibit structural defects [1] and their electronic and transport properties will be affected accordingly [2]. In addition, the presence of defects in carbon-based nanostructures has been seen as source of magnetism [3]. Hence, mastering the physics underlying defected CNTs is crucial not only to model realistic systems but also to design new devices.

The spin-polarized electron transport properties of carbon nanotubes with vacancies are investigated using first principles and non-equilibrium Green's function techniques [4]. Carbon atoms with unsaturated bonds are found to behave as quasi-localized magnetic impurities, coupled by long range interactions. The magnetism of carbon nanotubes with reconstructed mono- and tri-vacancies results in spin dependent contuctances and, hence, can be exploited in spintronic devices such as nano-spin valves.

Clarified the properties of CNTs with vacancies, the sensing ability of defected CNTs towards several molecules (NO$_2$, NH$_3$, CO, CO$_2$, H$_2$O) has also been investigated {it ab initio}. Since the adsorption/desorption of molecules induces modulations on the electrical conductivity of the tube, quantum conductances of the CNT-based sensors are predicted, finding that defective nanotubes are sensitive to NO$_2$, NH$_3$ and CO, while molecular selectivity is provided by the nature of the charge transfer.

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Nanomagnetic phenomena in transition metal nanowires

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Abstract

Magnetism in nanosystems is interesting since magnetic phenomena appear to be very sensitive to the dimensionality of the system. This means that metals which normally show no magnetism (not even as a free atom) can be provoked to spin-polarize if, for example, grown as a very thin surface, or formed into an extremely thin wire, a so-called nanowire. The thinnest nanocontacts between two metal bodies sometimes take the shape of regular ultra-thin suspended nanowires. I will qualitatively review here some of the theory work done in our group on transition metal nanowires. I will outline why magnetism may arise in nanowires, and how this magnetism may affect other physical properties, in particular the quantized conductance through the nanowire.
Further, the magnetic anisotropy is expected to be very large in low-dimensional systems, and our calculations show that this is indeed the case. In fact, in platinum wires, one could even speak about "colossal" magnetic anisotropy – the absolute impossibility of magnetization to rotate from parallel to orthogonal to the nanowire axis. Finally, I will discuss some preliminary results regarding the spin dynamics of nanowires.

Density Functional based calculations for nanostructures containing large numbers of atoms

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Spintronics with graphene nanoribbons

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Abstract

Over the past few years graphene has become one the most studied systems in nanoelectronics. The fact that nanostructured graphene (graphene nanoribbons, graphene dots, voids in graphene, etc.) can present magnetic order also makes it of interest for spintronics applications. I will discuss how the imbalance in the number of atoms belonging to the two graphene sublattices, the existence of zero-energy states, and the total and local magnetic moments are intimately related [1]. Magnetism thus becomes naturally associated with graphene nanoribbons terminated by zig-zag edges and nanoribbons with vacancies and adsorbates such as H, which opens interesting possibilities in spintronics for these systems [2,3]. With the help of the quantum transport package ALACANT [4], we explore various possibilities for the use of graphene nanoribbons as all-carbon based magnetoresistive devices.

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A quest for a molecular diode based on the mechanism of elastic scattering in asymmetric junctions

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Abstract

The quest for a molecular diode started by a famous proposal of Aviram and Ratner in 1974, so far did not bring an unquestionable success. Some recent estimates (see, e.g. [1-3]) using simple models and ab initio studies raised doubts whether it would be possible to obtain a sizable rectification coefficient in molecular junctions, at least based on the mechanism of elastic scattering.

Contrary to the most of the ab initio studies, using the trial and error
method by applying different molecules and various substitutions, in my talk I propose a way of a systematic study of the junctions, in which the asymmetry necessary for the molecule to act as a diode can be continuously varied by an application of a local external charge probe. The preliminary results using SMEAGOL program [4] do not bring however much improvement over the previous works and it seems important to consider other mechanisms of the diode type behaviour, like electron correlations or inelastic scattering.

In second part of my talk I will consider an alternative mechanism for obtaining a good molecular diode, using a cooperation of Coulomb correlations (e.g. [5,6]) and symmetry perturbations of a planar molecule. With a help of a simple parametric model (Hubbard Hamiltonian) to describe a triangular molecule [7,8] in the Coulomb blockade limit I will indicate the parameters' regime where the model molecule exhibits a

negative differential resistance behaviour as well as the high rectification ratio.

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(*) In cooperation with B. R. Bułka and the Lancaster SMEAGOL team: V. M. Garcia-Suarez, S. Bailey, C. Lambert.

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Generalization of Bardeen's transfer Hamiltonian method to include inelastic currents due to electron vibration coupling

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Abstract

Bardeen's transfer hamiltonian method is adequate to calculate tunnelling currents in the limit of weak tip-sample coupling. Therefore, it is well suited to describe many experimental observations done with the Scanning Tunneling Microscope (STM), except cases in which the tip-sample distance is close to contact. In this talk, I will present a simple and efficient way to implement this approach using a plane wave based DFT code, as well as results for the CO/Cu(111) benchmark system.
Next, I will describe a generalization to include inelastic currents due to electron vibration coupling. It is based on first order perturbation theory and, therefore, it is limited to weak electron-phonon coupling. However, it permits an efficient evaluation of the changes in conductance due to the opening of the inelatic channels in a large number points of a real space grid, which is very convenient to simulate topographies, conductance and vibrational maps, as measured in the experiments. Furthermore, the method permits to address problems in which the structure of the STM tip apex plays a role, like changes in the intensity of the inelastic signal due to different geometric structures or chemical termination. Other effects, like variations of the inelastic signal due to changes in adsorbate coverage will be discussed as well.

Bound and weakly coupled states in electron transport calculations

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Abstract

One of the challenges in applications of the non-equilibrium Green's functions formalism (NEGF) for electron transport calculations is the treatment of weakly coupled and bound states. While in some cases the standard NEGF formalism is not suited to treat such states, for many materials systems we can formulate a valid description. A formalism for the inclusion of bound states in the calculation of the non-equilibrium charge density within the NEGF method is outlined. Their occupation is set based on the assumption of an effective coupling of these states to the leads. This can usually be determined based on physical constraints, such as the geometrical location of a bound state inside a junction. We introduce the concept of generalized bound states, which allows us to describe both weakly coupled and bound states with a single formalism. We also present an efficient scheme to obtain an adaptive energy mesh for the integration of a highly resonant density of states over energy. This is one of the prerequisites of large scale simulations on systems with weakly coupled states. These methods are then applied to study the bias dependent transport through Fe/MgO/Fe tunnel junctions and through macromolecules.

Interplay of charging, conformation and magnetisation in metal (II) organic complexes: a DFT study

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Abstract

We investigate, how charging affects the high-spin/low-spin transition in Fe(II)-organic complexes. This transition is well studied in bulk materials where it can be driven by temperature, pressure or light. Our calculations employing the density functional theory (DFT) show that also charging with two electrons can induce the transition.
Calculations also indicate that a complex carrying a single excess charge is very close to a magnetic and geometric instability. In this state even moderate conformational changes could in principle trigger the spin transition. In transport experiments this behavior would manifest itself as a splitting of the Kondo resonance. Intriguingly, this may in fact have been already observed in recent experimental work by Anne Bernand-Mantel and Herre van der Zant (TU Delft, unpublished).

Incorporating Exchange-Correlation Effects in Quantum Transport through Nano-scale Junctions

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Abstract

State-of-the-art computational methods for modelling electron transport in nano-scale junctions are based on effective single- particle approximations such as the Kohn-Sham theory of density functional theory. This methodology has been successfully applied to junctions with strong coupling to the metallic electrodes, but has proved insufficient for less homogeneous junctions where the distinction between the nano-device and the electrodes is more pronounced. In order to obtain a more accurate and rigorous description of exchange-correlation effects in weakly correlated molecular junctions, we have implemented the many-body GW approximation within a transport framework suitable to treat non-periodic systems consisting of an interacting region coupled to infinite non-interacting leads with different chemical potentials. Fundamental trends in the properties of metal-molecule-metal junctions are identified on the basis of simple model calculations. These include renormalization of molecular QP levels due to dynamical polarization effects both in- and out of equilibrium as well as the reduction of QP life-times due to enhanced QP scattering under finite bias conditions. As will be shown, these genuine many-body effects can have a large influence on the junction IV characteristics even for weakly correlated systems. The

importance of using a fully self-consistent GW self-energy for quantum transport calculations will be demonstrated. Finally (preliminary) results for more realistic molecular junctions will be discussed.

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Microscopic Modelling of charge transport in molecular crystals, polymers and liquid crystals

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Electron-vibration couplings in single-molecule junctions

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Abstract

In this presentation I will describe methods based on the SIESTA and TranSIESTA density-functional schemes to calculate electron-vibration couplings and to simulate and analyze their influence on the transport properties of nanoscale junctions [1,2].

Special focus will be on the transport through single C60 molecules between metallic contacts in two different limits of the coupling to the electrodes: (i) When the coupling is sufficiently weak, the molecular levels are well-resolved in energy. In this case the tunneling
electrons explore vibronic molecular states with interesting features arising from the Jahn-Teller effect [3]. (ii) When the coupling is stronger, the molecular levels hybridize with the electrode states, and inelastic signals arise from phonon emission during the tunneling events. Using an eigenchannel analysis we characterize the propensity rules for the vibrational modes.

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NON-EQUILIBRIUM GREEN's FUNCTIONS AND DENSITY FUNCTIONAL TIGHT-BINDING: A CRITICAL REVIEW AND PERSPECTIVES OF FUTURE DEVELOPMENT

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Abstract

Molecular electronics is still a fascinating concept, attracting the interest of the scientific community thanks to the challenges it poses at experimental as well as fundamental theoretical level. The quantum transport tool based on the efficient density functional tight-binding (DFTB), that we have developed over several years has now reached a good level of maturity [1].
Coherent transport in nanojunctions and multiterminal systems as well as incoherent transport and power dissipation has been implemented in the non-equilibrium Green's function framework [2-4].
The current status of our approach will be reviewed, discussing the strengths and weaknesses of its main approximations and showing recent applications to transport in molecular transistors, heat dissipation in molecular junctions and the role of surface defects in inorganic Si nanowires [5-6].
The method will be put in perspective as part of a novel hierarchical approach for the description of modern nanostructured devices, spanning from density functional to empirical tight-binding up to continuous models based on finite elements that we are developing in our group [7].

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Electron transport across locally magnetic nanocontacts

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Abstract

Nanocontacts made of two nonmagnetic leads bridged by some magnetic structure are presently of considerable interest because of a variety of possible phenomena such as spin filtering, anisotropic magnetoresistance, low temperature Kondo physics and so on. The magnetic bridge may consist of a transition metal impurity or may even consist of the same metal as the leads, turning spontaneously magnetic as expected for Pd or Pt [1]. We will discuss both cases, the second exemplified by a Pt nanowire contact, and the first by a Ni impurity on a Au chain (representing the leads). Electronic structure, ballistic conductance, and impurity phase shifts were calculated using the standard Density Functional Theory (DFT) plane wave package Quantum-ESPRESSO [2].

In the case of Pt nanocontacts, we find that short segments of Pt atomic chains remain magnetic (with an easy axis along the nanowire) even if in contact with nonmagnetic Pt leads [3]. The calculated static Landauer-Buttiker conductance can only be reconciled with experimental data if local magnetism is included.

In the case of Au nanowire with a Ni impurity, we find that the magnetic moment of the Ni atom depends dramatically on the impurity site geometry [4], changing from $1 \mu_B$ in the bridge geometry to $2 \mu_B$ in the substitutional one. Moreover, the sign of the effective exchange coupling between the spins of conduction electrons and that of the Ni impurity is antiferro (predicting a regular Kondo effect) in the bridge case, but ferro (predicting local moment formation) in the substitutional one. These Kondo phenomena are investigated by building appropriate Anderson models which reproduce the DFT phase shifts and which are solved via Numerical Renormalization Group [5]. Predictions are made for the zero-bias conductance anomalies, very different in the two cases.

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Tilt angle dependence of electronic transport in molecular junctions of self-assembled alkanethiols

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Abstract

Measurements done using conductive scanning force microscopy under low load conditions permit to obtain reliable tilt angle and molecular length dependences of the low bias conductance through the alkanethiol molecular layers. We use several well-characterized self-assembled structures of alkanethiol molecules on Au(111) where molecules present a different angles with respect to the surface normal. The observed tilt-angle dependence of the conductance is stronger for the longer molecular chains and, therefore, would suggest the importance of intermolecular (through space) tunneling pathways.

To model this system we have performed first-principles calculations of the transport through monolayers of alkanedithiols between two Au(111) electrodes. The tilt angle dependence of the calculated conductance is similar to that observed experimentally. We use our theoretical results to analyze in detail the different mechanisms contributing to the observed behavior.

Interference effects and Fermi level alignment in electron transport through nitro-benzene nano-junctions

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Abstract

Electron transport between nanoscale contacts has become a much debated field in the last few years, due to its possible applicability in molecular electronics and recent progress in its experimental characterisation. Recently, interest in employing quantum interference effects (QIE) for the design of single molecule devices has considerably intensified [1]-[8]. Such effects occur when electron waves pass through nano junctions phase coherently and depend crucially on symmetry. For making use of QIE and its influence on electron transport properties as an enabling tool for single molecule devices two conceptually different proposals have been brought forward: i) In a QIE transistor tunable coherent current suppression can be achieved by applying a local electric field or gate potential to an aromatic molecule covalently bonded to source and drain electrodes, where the operating principle is introducing decoherence or dephasing to the electron transmission between the leads [1],[6]-[8]. ii) Another way of taking advantage of QIE for molecular electronics lies in controlling electron transmission by chemically modifying or changing the conformation of side groups to aromatic molecules, which has been suggested as a concept

for data storage [2], the implementation of intra-molecular logic gates [3] or single-molecule sensors [5]. In our paper we focus on the side group proposal for QIE. We present density functional theory (DFT) based non-equilibrium Green's function (NEGF) calculations for the conductance through a nitrobenzene molecule, which is anchored by pyridil-groups to Au electrodes. This work is building up on earlier theoretical studies where quantum interference effects have been identified both in qualitative tight-binding (TB) [2],[3] and in DFT descriptions for the same molecule with different chemical connections to the leads [4]. The novelty in the current contribution is two-fold: i) the pyridil-anchors guarantee for the conductance to be determined by rather narrow peaks situated closely to the Fermi energy which maximizes the impact of quantum interferences on the I/V behaviour and helps to make them accessible to experiments, ii) a semi-quantitative comparison between TB models and DFT results for the investigated systems aims at facilitating the chemical design of nano-electronic devices based on quantum interference effects controlling the electron transport through single molecules.

While QIE affects the shape of the transmission function, the second theme of the presentation is Fermi level alignment and its relation to charge transfer [9]-[14]. This later feature determines the relative positioning of the peak structure in the transmission function with respect to the Fermi energy of the metal electrodes. It has to be analyzed in terms of the filling/emptying of molecular levels combined with Pauli repulsion effects [9] and has been shown to depend strongly on the details of the surface structure [10] and metal type [12] of the electrodes as well as molecular structure [14]. We show and explain how nitro-groups affect the level alignment of pyridil-anchored benzene, and put particular emphasis on the differences between nitro-benzene with a para- and meta-connection of the pyridil-anchors and also on the influence of the torsion angle between the aromatic rings.

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Controlling transport properties by molecular structure and light

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Abstract

Transport properties of organic molecules can be controlled via the molecular structure [1]. We consider the characteristic changes of conductance and thermopower at the example of oligophenylenes [2,3,4]. Beside changing the number of ring units, side groups may be attached, and both conformational as well as electron-donating effects may play a role. In particular, we discuss the temperature-dependent conductance of biphenyl molecules [2] and demonstrate a linear behavior of the thermopower as a function of molecular length [3,4], as observed recently [5,6]. As time permits, we will present studies on the photoconductance

[3,7].

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Strong Correlations in Quantum Dots and Wires: Quantum Monte Carlo Studies

Harold Baranger
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Abstract

Nanostructures provide unprecedented control and access to a variety of strongly correlated electronic states. I shall present quantum Monte Carlo (QMC) results on two examples.
(1) Transport spectroscopy of Kondo correlations in a box-- Motivated by experiments on double quantum dots, we study the problem of a single magnetic impurity confined in a finite metallic host. Analytic arguments and path-integral QMC results for weak to strong coupling map out the spin excitations that can be probed in simple tunneling-spectroscopy transport [1, 2]. We explore the possibility of using QMC techniques to calculate the conductance through a Kondo correlated quantum dot.
(2) Interaction-induced localization in an inhomogeneous quantum wire-- We study the localization of electrons induced by electron-electron interactions in an inhomogeneous 1D system: a wire with two regions, one at low density and the other high [3]. QMC results show that the electrons become localized if the density is sufficiently low. We focus on the separation between the high density and low density regions. If the external potential changes abruptly at the interface, a barrier develops between the two regions, causing Coulomb blockade effects. For a short low density region, as in a quantum point contact, a single localized electron naturally occurs. The picture emerging here is in good agreement with the experimental measurements of tunneling between two wires (the Yacoby group), and has implications for the "0.7 anomaly" in the conductance of quantum point contacts.

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Transport in graphene layers connected by carbon nanotubes

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Abstract

The study of electronic transport both in graphene and in carbon nanotubes has attracted a great deal of work, due to the interesting fundamental phenomena that these materials display and to the promise of outstanding applications in nanoelectronics. The two- and one-dimensional character of the two materials, respectively, confer them with sharply different electronic transport properties, and therefore different potential applications are envisioned.

In this work, we have considered the possibility of future devices that may use combinations of graphene layers and carbon nanotubes for electronic applications. For instance, nanotubes might be used to transmit electronic signals between two graphene-based devices, in the same way as copper wires do between traditional silicon-based transistors.

We present first-principles studies of the transport properties of a system consisting on two graphene sheets connected by a carbon nanotube. We consider different nanotubes with different chiralities and lengths, and also different types of connections between the tube and the sheet. We compute the ballistic transport between the two sheets through the nanotube, and show that the behavior of the conductance is qualitatively different for metallic and semiconducting nanotubes. We also show how the conductance depends on the link between the nanotube and the graphene sheet.

Kadanoff-Baym dynamics in strongly correlated nanostructures
Carl-Olof Almbladh
Physics Department, Lund university

Software demonstration from QuantumWise A/S
Kurt Stokbro
University of Copenhagen, Denmark

5 Poster list

Conductance of alkanedithiol single-molecule junctions: a molecular dynamics study

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Abstract

We study the formation and conductance of alkanedithiol molecular wire junctions using density functional based molecular dynamics and non-equilibrium Green's function techniques. The stretching of the junction involves straightening of the wire, migration of thiol end-groups on the Au contact surfaces and Au atoms being pulled out. The low-bias conductance traces show clear plateaux associated with a single molecule bridging the electrodes. In situations where the molecule contains a gauche defect we find that the conductance plateau is decreased by approximately one order of magnitude. In contrast, the weaker dependence on the conductance of the Au-S coordination is hidden in thermal noise at 300 K. Calculated inelastic electron tunnelling spectra further show clear effects of the junction geometry thus providing additional clues to distinguish between different microscopic configurations of individual molecular wires. In particular, our simulations suggest ways to identify gauche defects in transport measurements.

The role of electron-phonon interactions in the tunnelling regime

Eunan McEniry
Queen's University Belfast

Abstract

The role of electron-phonon interactions in the tunnelling regime is investigated. Through application to a model tunnelling system, it is illustrated analytically that second-order electron-phonon coupling provides a contribution to the effective transmission function which is of the same order as the conventional linear approximation. The correlated electron-ion dynamics is compared with standard non-equilibrium Green's function theory, and applied to a number of model tunnelling systems. The divergences in the results are discussed, and explained partially by the explicit inclusion of higher-order electron-ion coupling terms in the dynamical approach, which are absent from the Green's function procedure.

Ballistic Transport in 1D Systems using Wannier Functions obtained within the FLAPW Method

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Abstract

We report the development of a ballistic transport code for one-dimensional magnetic systems based on Wannier functions (WF) constructed within the full-potential linearized augmented plane-wave (FLAPW)

method). We describe the details of the construction of first-shot (fsWF) or maximally localized (MLWF) WFs from the FLAPW wavefunctions choosing a monoatomic Pt chain as a model system. For the calculation of ballistic transport, we apply the Landauer formalism using Green's functions. The Hamiltonian of the system including a scattering region attached to semi-infinite leads is constructed from the WFs which serve as a localized basis set. We discuss different coupling techniques of the scattering region to the leads. The open boundary conditions are treated by replacing the leads by their self-energies obtained via the decimation technique. From the Green's functions we can immediately calculate the conductance of the system. As a first application of the approach, we study the transition from the contact to the tunneling regime in monoatomic Pt wires, as well as in ferromagnetic Co monowires of parallel and antiparallel alignment. Furthermore we investigate the effect of spin-orbit coupling (SOC) on the transmission of such a Pt monowire with one stretched bond.

Adsorption of CO on monatomic wires: a comparison between Pt and Au

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Abstract

Recent experiments addressed the eect of a CO molecule on the ballistic conductance of Au, Cu, Pt and Ni atomic contacts, showing that the molecule modi es the break junction conductance histograms in a peculiar way for each metal[1]. CO interacts both with Pt and Au nanojunctions, but the changes in the histograms look very dierent for the two metals and lack of a comprehensive interpretation. We investigate the electronic structure and ballistic conductance of these systems by studying, within density functional theory, an idealized model made of one CO molecule adsorbed on an in nite straight monatomic chain of platinum [2] or gold. We compare the two metals and study the eect of the CO adsorption site (top or bridge) on the ballistic conductance. We nd that, for both Pt and Au, the molecule prefers to attach at the bridge site of the chain and that the binding involves a Blyholder-like donation/back-donation mechanism between the molecule and the metal. The transmission of s electrons is characterized by some dips at speci c energies which depend on the details of the interaction, which in turn depends on the metal, on the adsorption site and also on the strain of the wire. Spin-orbit coupling influences substantially the band structures of Pt and Au chains, but perturbs only slightly these features. If these dips appear at the Fermi energy, a strong reduction in the conductance is expected for the Au chain, where only s electrons are present at that energy. Actually this happens for a strained con guration with CO ontop (as previously found by others [3]), and can be directly related to the donation of molecular g states. However, a smaller strain or a dierent adsorption site can spoil this effect and restore larger values of conductance. The study of the eects of more realistic atomic con gurations (a short wire between tips/surfaces) on these conclusions is in progress.

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Adverse effects of asymmetric contacts on single molecule conductances

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Abstract

We find that for molecular wires with mixed functional groups (X–bridge–Y) the single molecule conductance decreases with respect to the comparable symmetric molecules [1]. These differences are confirmed by theoretical computations based on a combination of density functional theory and the non-equilibrium Green's functions formalism. This study demonstrates that the apparent contact resistance, as well as being highly sensitive to the type of the anchoring group, is also strongly influenced by contact-asymmetry of the single molecular junction which in this case decreases the transmission. This highlights that contact-asymmetry is a significant factor to be considered when evaluating nanoelectrical junctions incorporating single molecules.

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Impact of dimerization and stretching on the transport properties of molybdenum atomic wires
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Abstract

We study the electrical and transport properties of monoatomic Mo wires with different structural characteristics. We consider first periodic wires with inter-atomic distances ranging between the dimerized wire to that formed by equidistant atoms. We find that the dimerized case has a gap in the electronic structure which makes it insulating, as opposed to the equidistant or near-equidistant cases which are metallic. We also simulate two conducting one-dimensional Mo electrodes separated by a scattering region which contains a number of dimers between 1 and 6. The $I - V$ characteristics strongly depend on the number of dimers and vary from ohmic to tunneling, with the presence of different gaps. We also find that stretched chains are ferromagnetic.

Density-functional theory study of transmission channel degeneracy and thermopower in biphenyl based single molecules junctions
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Abstract

Using density-functional theory, we investigate the charge transport properties for a series of recently synthesized biphenyl molecules [Mishchenko et al., submitted]. The molecular conformation, i.e. the twist angle varphi between the two phenyl rings, and hence the degree of pi conjugation is controlled by alkyl chains and methyl side groups. We study two linker groups, thiols and amines, and consider three different bonding geometries, hollow-hollow, bridge-bridge and top-top. We find that the conformation inside the metal-molecule-metal junction can strongly differ from those for the gas-phase molecules, especially for the thiols.

The different bonding geometries and linkers give rise to conductances, which vary by one order of

magnitude for the same molecule, which we explain by the different hybridization of molecules with electrode orbitals. Irrespective of considered linker groups and geometries we find a cos^{2}varphi dependence of the conductance. We study the transmission channels, which contribute to the conductance, and observe that for all molecules, except for those with completely broken conjugation, the transmission is dominated by one channel, formed from the pi electrons. For perpendicular rings, we observe a degeneracy of two transmission channels for the symmetric hollow-hollow geometries due to sigma -pi coupling. However, for the other less symmetric geometries, this degeneracy is lifted. Similar to the conductance, we find also the thermopower to depend strongly on the bonding positition and the linker. The results confirm a weak cos^{2}varphi variation, proposed previously

Analyzing Capacitance-Voltage measurements of vertical wrapped-gated nanowires

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Abstract

The capacitance of arrays of vertical wrapped gate InAs nanowires has been measured. With the help of a Poisson-Schrodinger solver various features of the collected data can be explained and comparison with the theoretical model furthermore enables us to determine the concentration of dopants. Once this concentration is determined the surface state density can be estimated by analytical means. The model is also used to evaluate the doping concentration required for the coexistence of electrons and holes. It is furthermore shown that the dierence between the actual capacitance and the geometrical limit is quite large, and depends strongly on the nanowire material.

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The maximum entropy principle and the DC molecular transport

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Abstract

A few years ago, Delaney and Greer [1] claimed that a variational many-body method based (i) on the maximum entropy principle [2] and (ii) expressing the boundary conditions by using the Wigner function is able to correctly reproduce the steady-state current through correlated molecules like benzene-dithiol. To check its theoretical background, we have implemented the linear response approximation exactly as proposed in Ref. 1, and applied it to calculate the zero-bias conductance of a single-electron transistor both without (U=0) and with (U≠0) correlations [3]. The results unambiguously demonstrate that this method

yields in both cases a completely unphysical behavior. To better understand the failure of this approach, we have relaxed the boundary conditions and considered, instead of the Wigner function, general boundary conditions [4]. The analysis shows that even by imposing boundary conditions in terms of the Fermi distributions in electrodes, which are ubiquitously employed in transport theories, the approach is invalid, as it unphysically predicts a vanishing zero-bias conductance. Therefore, we must conclude that the maximum entropy principle applied to a system described by a unique wave function, as done in Ref. 1, is unable to describe the steady-state current.

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Andreev reflection through Fano resonances in molecular wires

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Abstract

We study Andreev reflection in a normal conductor-molecule-superconductor junction using a first principles approach. In particular, we focus on a family of molecules consisting of a molecular backbone and a weakly coupled side group. We show that the presence of the side group can lead to a Fano resonance in the Andreev reflection. We use a simple theoretical model to explain the results of the numerical calculations and to make predictions about the possible sub-gap resonance structures in the Andreev reflection coefficient.

Molecular vibrational spectroscopy from tunneling to contact

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Abstract

Within the field of molecular nanojunctions, a detailed understanding of the evolution of inelastic transport properties as junctions are tuned from tunneling to contact is vital for their future ultimate application to molecular electronics nanotechnology. We present IETS (inelastic electron tunneling spectroscopy) spectra of CO molecules on Cu(111) for tip-molecule distances ranging from tunneling to contact regimes, which allows tracing the evolution of the inelastic signals. In tunneling conditions, the dominant signal at ~ 35meV is associated to the frustrated rotation of the CO molecule. Surprisingly, this signal is strongly shifted to ~ 28meV as the tip approaches contact. This scenario has been successfully reproduced by detailed theoretical calculations of the vibrational modes and of the corresponding inelastic transport spectra. Our calculations are in very good agreement with experiments and could explain the experimental shift of the inelastic signal as originated by the molecule-tip interacion.

Effect of the Chemical Functionalization on Charge Transport in Carbon-Based Materials at the Mesoscopic Scale

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Abstract

The chemical attachment of groups on single-walled carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) has attracted much attention as it provides an efficient way for tuning their electronic properties. These carbon-based systems are being widely investigated as potential candidates for nanoelectronic interconnects and transistors. The control of electric current is, therefore, an important challenge in nanostructures engineering[1].

Here we present a theoretical methodology and study of charge transport through GNRs [2], as well as in metallic and semiconducting CNTs [3], with randomly distributed functional groups covalently attached to the system surface. We resort to both first principles calculations, to obtain a suitable parametrization of the electronic structure, and a fully ab initio transport approach calculation to explore conduction regimes through large and disordered systems. The quantum transport modeling is based on the Green's function formalism, combining an iterative scheme for the calculation of transmission coefficients with the Landauer's formula for the coherent conductance.

Our results describe how the conductance of the hybrid systems is altered as a function of incident electron energy and molecules coverage density. We explore the transport regimes comparing two different types of functional groups. Phenyls and hydroxyl groups induce a local rehybridization from sp2-type to sp3-type orbital of the carbon atoms yielding a localized transport regime. On the other hand, carbene groups do not disrupt the original sp2 network which allows a good conductance preservation.

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Inhomogeneous Hubbard model in the Gutzwiller approximation

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Abstract

This poster was motivated by recent ARPES measurements of Rodolakis et al.[1], showing the decay of quasiparticle weight away from the crystal surface of a strongly correlated V2O3 crystal close to the Mott transition. The simplest model we can use for such a system is an open-boundary, inhomogeneous-U Hubbard model. We present therefore a Gutzwiller description of the inhomogeneous-U Hubbard model at half filling [2]. The electronic Hamiltonian, which depends on a set of site-dependent parameters describing the renormalization of hopping and double occupation probability, is diagonalized exactly. The

optimization with respect to the parameters is instead performed by means of an iterative map, converging to a fixed point in parameter space. The Gutzwiller analytical expression [3] for the hopping renormalization is known to be exact in infinite-coordination lattices [4], while it is considered an approximation in finite coordination lattices. We apply this method to a couple of different inhomogeneous-U geometries other than the crystal-surface, like a metal-strongly correlated metal junction and a metal-Mott insulator-metal junction.

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First-Principles conductance of nanoscale junctions from the polarizability of finite systems

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Abstract

We derive an expression for the 4-point conductance of a general quantum junction in terms of the density response function. The method for the calculation of the conductance of nanoscale electrical junctions is used within ab-initio electronic structure methods which make use of the periodic supercell technique, and applied to realistic models of metallic wires and break-junctions of sodium and gold. The method is systematically controllable and convergeable, and can be straightforwardly extended to include more complex processes and interactions.

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