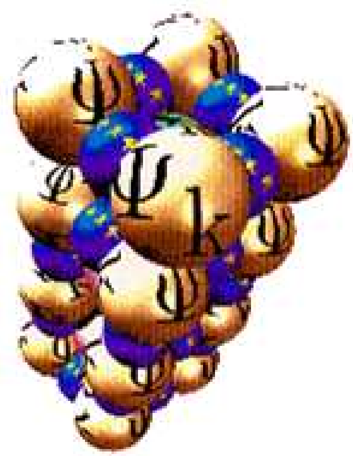
Ψ_k Newsletter

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 80 April 2007



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Contents

1 Editorial

In this second Psi-k newsletter of 2007, we would like to turn our readers attention to a very impressive scientific highlight by G. Brocks, V. M. Karpan, P. J. Kelly, P. A. Khomyakov, I. Marushchenko, A. Starikov, M. Talanana (University of Twente, The Netherlands), I. Turek (Academy of Sciences of the Czech Republic, Brno), K. Xia (Chinese Academy of Sciences, Beijing), P. X. Xu (University of Twente, The Netherlands), M. Zwierzycki (Polish Academy of Sciences, Poznan), G. E. W. Bauer (Delft University of Technology, The Netherlands) on "Calculating Scattering Matrices by Wave Function Matching". For other items of the newsletter please check the table of contents.

The *Networks* have a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

http://psi-k.dl.ac.uk/

The above contains information on the Psi-k 2006/2007 workshops and hands-on courses (subject to funding).

Please submit all material for the next newsletters to the email address below.

The following email addresses, which remain in operation, are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@dl.ac.uk	**messages to the coordinators, editor & newsletter**
psik-network@dl.ac.uk	**messages to the whole Ψ_k community**

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2 News from the ESF Programme

”Towards Atomistic Materials Design”

2.1 Reports on ESF Psi-k Workshops/Conferences

2.1.1 Report on Workshop ”Quantum Transport and non-adiabatic electron evolution from first principles approaches”

CECAM - Lyon (France)

December 4-8, 2006

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The workshop was extremely lively and worthwhile, with much discussion and exchange of ideas. From the amount of new work presented, it was clearly timely, and the field is obviously still in a state of flux. The meeting of two communities (roughly characterised by their interest in different areas: either molecular electronics and narrow constrictions, or layered materials and spin transport) was profitable as it allowed the mixing of ideas and assumptions from each area.

One of the topics addressed was the calculation of transport from DFT in both communities (using Landauer approach and both scattering and non-equilibrium Green’s function formalisms). This overall framework is becoming well-understood, but it is clear that there are still considerable efforts underway in the areas of efficiency and implementation. However, in a way, the workshop has established that, despites differences in the technical details of particular implementations, the basic formulation for transport based on DFT is well established and commonly accepted by both communities, who have arrived in parallel to essentially the same conceptual framework. In that sense, it seems that the workshop has arrived at a late moment, and that if it would have taken place some time ago, it would probably have had a larger impact in the development of both communities.

Going beyond these standard techniques was a major concern of the workshop. The two main topics were going beyond DFT (more accurate techniques such as GW, CI, and TDDFT to allow more precision in the calculation of the electronic structure), and including non-adiabatic effects (allowing the electronic subsystem to couple to the phononic subsystem to exchange energy). While there have been steps forward in both these areas, they are in their infancy, and the best ways to proceed are not clear. These are lines which will most probably develop quickly in the near future.

The fact that DFT approaches coupled to Non-Equilibrim Green's Functions techniques have become standard in dealing with transport problems, has lead to the community to a deep discussion of what are the limitations, deficiencies and basic flaws of these approaches. Hints on the inability to describe common effects such as Coulomb blockade have become apparent, and the basic reasons unraveled. Approaches to solve these deficiencies are being proposed. Ultimately, methods based on sound foundations like TDDFT appear to be promising, at least to understand the origin of the flaws of the standard approaches. Converting them into practical, accurate and predictive tools which can be applied to real problems is one of of the main challenges for the future.

An important conclusion of the workshop was the need to find experimental validation for the quality of present-day calculations. While accurate and reliable experimental results in well controlled systems are widely available in the field of transport in solid state layered systems, the situation in the molecular electronics area is very different. There, the dispersion in the experimental results is very large (sometime, with orders of magnitude difference), as well as the difference between theory and experiment (especially in the low-conductance regime). Having well controlled, reproducible experimental results would be extremely useful for the simulation community, in order to establish the validity and accuracy of the computational techniques.

Program

Day 1: Dec. 04 2006

Session : 0 Welcome and Foreword
08:50 to 09:00 : Welcome

Session : 1 Transport in the Linear Response Regime (I)
09:00 to 09:45 : Presentation
First-principles scattering matrices for spin-transport
Maciej Zwierzycki

09:45 to 10:30 : Presentation

Multilayer transport calculations within the CPA including vertex corrections

Karel Carva

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation

Finite element implementation of NEGF for nanostructures

Martti Puska

11:45 to 12:30 : Presentation

Electronic transport through Wannier functions: from molecular to solid state systems

Arrigo Calzolari

12:30 to 14:00 : Lunch Break

Session : 2 Transport in the Linear Response Regime (II)

14:00 to 14:45 : Presentation

All-electron calculations of electronic transport: applications to magnetic tunnel junctions

Daniel Wortmann

14:45 to 15:30 : Presentation

Electronic transport through quantum wires and tunnel junctions: a real-space finite-difference approach

Petr Khomyakov

15:30 to 16:00 : Coffee Break

16:00 to 16:45 : Presentation

Korringa-Kohn-Rostoker Green-function formalism for ballistic transport

Phivos Mavropoulos

16:45 to 17:30 : Presentation

Computing conductances by layer-KKR: from planar tunnel junctions to STM

Jü rgen Henk

17:30 to 18:00 : Discussion

18:00 to 19:00 : Poster Session

Day 2: Dec. 05 2006

Session : 1 Non Equilibrium Green's Functions Approaches
09:00 to 09:45 : Presentation
Ab-initio TB-LMTO method for nonequilibrium electron transport in nanosystems
Sergey Faleev

09:45 to 10:30 : Presentation
The TranSIESTA/ATK method
Jeremy Taylor

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation
Strong correlation and order-N in quantum transport: the Smeagol project
Stefano Sanvito

11:45 to 12:30 : Presentation
Nanoelectronics with ALACANT: Fundamentals and applications
Juan José Palacios

12:30 to 14:00 : Lunch Break

Session : 2 Spin Transport (I)
14:00 to 14:45 : Presentation
First-principles scattering matrices in magnetoelectronics
Gerrit E. W. Bauer

14:45 to 15:30 : Presentation
Ferroelectric and Multiferroic Tunnel Junctions
Evgeny Tsymbal

15:30 to 16:00 : Coffee Break

16:00 to 16:45 : Presentation
Efficient spin injection from a ferromagent into a semicondutor
Volodymyr Karpan

16:45 to 17:30 : Presentation
First-principles calculations of spin-dependent tunneling and spin-disorder resistivity
Kirill Belashchenko

17:30 to 18:00 : Discussion

18:00 to 19:00 : Poster Session

Day 3: Dec. 06 2006

Session : 1 Non-adiabatic effects
09:00 to 09:45 : Presentation
First principles description of inelastic transport in atomic and molecular wires
Magnus Paulsson

09:45 to 10:30 : Presentation
Open boundaries and the CEID formalism
David R. Bowler

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation
Correlated Electron-Ion Dynamics in molecular systems
Andrew Horsfield

11:45 to 12:30 : Presentation
Time-domain ab initio studies of ultrafast excitation dynamics in nanomaterials
Oleg Prezhdo

12:30 to 14:00 : Lunch Break

Session : 2 Beyond NEGF DFT
14:00 to 14:45 : Presentation
The flow of molecular orbitals driven by gate or bias voltage in transport calculations based on density functional theory
Ferdinand Evers

14:45 to 15:30 : Presentation
Avoiding self-repulsion in density functional description
Roi Baer

15:30 to 16:15 : Presentation
Sources, sinks and correlations in electron transport
Giorgos Fagas

16:15 to 16:45 : Coffee Break

16:45 to 17:30 : Presentation

GW approach to quantum transport in nano-scale contacts

Kristian Thygesen

17:30 to 18:15 : Presentation

Linear response formalism for conductance of planar junctions

Peter Bokes

18:15 to 19:00 : Presentation

Hydrodynamic approach to transport in nano-systems

Roberto D'Agosta

19:00 to 20:00 : Discussion

Day 4: Dec. 07 2006

Session : 1 Spin Transport (II)

09:00 to 09:45 : Presentation

Interface resistance calculated from first principles approaches

Ke Xia

09:45 to 10:30 : Presentation

Spin-transport calculations in magnetic materials with presence of spin-orbit coupling and disorder

Anton Starikov

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation

High TMR ratio in Fe/MgO/Fe junctions with even one atomic Fe layer

Peter Zahn

Session : 2 Molecular Electronics

11:45 to 12:30 : Presentation

The physics and chemistry of molecular devices for moletronics and for the post CMOS era

Jorge Seminario

12:30 to 14:00 : Lunch Break

14:00 to 14:45 : Presentation

Applications of the Smeagol code to atomic and molecular junctions
Jaime Ferrer

14:45 to 15:30 : Presentation
First-principles calculation for electron conduction properties using real-space finite-different method
Tomoya Ono

15:30 to 16:15 : Presentation
Conductance, surface traps and passivation in doped silicon nanowires
Marivi Fernandez-Serra

16:15 to 16:45 : Coffee Break

16:45 to 17:30 : Presentation
Impurities in atomically-thin metallic nanowires
Frederico Novaes

17:30 to 18:15 : Presentation
Quantum Transport in Post-CMOS Molecular Materials & Devices :
Stefan Roche

18:15 to 19:15 : Discussion

Day 5: Dec. 08 2006

Session : 1 Time Dependent DFT Approaches
08:30 to 09:15 : Presentation
Long-time dynamics of the Kohn-Sham system for open molecular junctions
Gianluca Stefanucci

09:15 to 10:00 : Presentation
Time-Dependent Transport Phenomena: Transients, Pumping and the Role of Bound States
Stefan Kurth

10:00 to 10:45 : Presentation
Classical Nuclear Motion in Quantum Transport
Claudio Verdozzi

10:45 to 11:15 : Coffee Break

11:15 to 12:15 : Discussion

12:15 to 12:20 : Closing word

Abstracts

Linear response formalism for conductance of planar junctions

Peter Bokes

Slovak University of Technology, Slovakia

Abstract

In a need for self-consistent and beyond DFT-motivated approaches we reconsider the very definition of conductance of quantum junctions. Time-dependent simulations of establishment of the steady state with uniform current for simple model systems lead us to an observation that it is a 4-point conductance that can be unambiguously addressed within ab-initio methods [1]. This is particularly important for planar junctions where the differences between a usual 2-point conductance and the 4-point conductance are most severe [2]. We show how the 4-point conductance can be obtained from linear response functions and how it is affected with a general non-local exchange-correlation kernel within the time-dependent density-functional theory [3]. Beyond the linear response, the 4-point measurement motivates various current-constraining theories [4] that attempt to give a variational principle for the non-equilibrium steady-state density matrix. The latter will be briefly reviewed with emphasis on their merits as well as weaknesses.

References

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[3] P. Bokes, J. Jung, and R. W. Godby, cond-mat/0604317, submitted (2006).

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Time-Dependent Transport Phenomena: Transients, Pumping and the Role of Bound States

Stefan Kurth

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Abstract

The Landauer formalism is a popular method to calculate the current through a nanoscopic system connected to two (or more) macroscopic electrodes and, in combination with techniques of density functional theory, is now widely used to compute current-voltage characteristics of single molecules. However, the Landauer formalism has two main limitations: first, the electrons are treated as non-interacting particles and second, only the steady-state currents are accessible in this formalism. Both of these limitations can be overcome by using timedependent density functional theory.

Here we present a description of transport based on the time evolution of the non-interacting time-dependent Schrö dinger equation. We develop a numerical algorithm for the time propagation of extended states which is ideally suited for implementation of time-dependent density functional theory. We use the algorithm to study time-dependent transport phenomena such as transients in simple model systems. We investigate electron pumps where a pump current is produced between two unbiased electrodes by applying a periodic bias to a third gate electrode. We also comment on the role of bound states in transport which may lead to current oscillations that remain undamped even in the long-time limit.

GW approach to quantum transport in nano-scale contacts

Kristian Thygesen

Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark, Denmark

Abstract

Correlation effects within the GW approximation have been incorporated into the Keldysh non-equilibrium transport formalism. We show that GW describes the Kondo effect and the zero-temperature transport properties of the Anderson model fairly well. Combining the GW scheme with density functional theory and a Wannier function basis set, we illustrate the impact of correlations by computing the I-V characteristics of a hydrogen molecule between two Pt chains. Our results indicate that self-consistency in the GW self-energy is fundamental for transport calculations.

References

cond-mat/0609223

Computing conductances by layer-KKR: from planar tunnel junctions to STM

Jü rgen Henk

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Abstract

Regarding electronic transport as a scattering process, as in the Landauer-Bü ttiker theory, it appears obvious to compute conductances of nanoscale devices within the framework of multiple-scattering theory. In this presentation I introduce different approaches to conductance calculations by the layer Korringa-Kohn-Rostoker (layer-KKR) method. These base either on wavefunctions or on Green functions, both having specific advantages and disadvantages. For instance, planar tunnel junctions are treated by wavevector-resolved methods. The time-consuming Brillouin-zone integration is drastically reduced by adaptive-mesh algorithms. For STM, a real-space approach and its problems are discussed. Each method is briefly illustrated by an application.

Electronic transport through quantum wires and tunnel junctions: a real-space finite-difference approach

Petr Khomyakov

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Abstract

Nanoelectronics is a fast developing field. Therefore understanding of the electronic transport at the nanoscale is currently of great interest. We aim at a general theoretical treatment of coherent electronic transport in mesoscopic and microscopic systems by means of Green's function and mode-matching techniques [2]. Firstly, we show how all the Green function results can be derived from the mode-matching technique. A more compact expression for the transmission matrix elements is derived. Secondly, we present a general approach for conductance calculations, which is based upon Landauer-Buttiker formalism and the mode-matching technique within the real-space high-order finite-difference scheme for representing the single particle equation and wave functions [1]. Testing of this real-space finite-difference approach is done for model tunnel junctions. This approach in combination with the density-functional formalism is applied to the conductance calculations in monatomic wires. The entire system consisting of the wire and the semi-infinite electrodes, is treated fully atomistically. We study the oscillating behavior of the conductance as a function of the number of atoms in the wire. We focus on investigating the stability of even-odd conductance oscillations in monatomic sodium wires with respect to structural variations [3]. Important technical details affecting the conductance calculations are emphasized.

References

[1] P. A. Khomyakov and G. Brocks, Phys. Rev. B 70, 195402 (2004).

[2] P. A. Khomyakov, G. Brocks, V. Karpan, M. Zwierzycki, and P. J. Kelly, Phys. Rev. B 72, 035450 (2005).

[3] P. A. Khomyakov and G. Brocks, Phys. Rev. B 74, 165416 (2006).

Interface resistance calculated from first principles approaches

Ke Xia

The Chinese Academy of Sciences, China

Abstract

As devices are reduced in size, interfaces start to dominate electrical transport making it essential to be able to describe reliably how they transmit and reflect electrons. For a number of nearly perfectly lattice-matched materials, we calculate from first-principles the dependence of the interface transparency on the crystal orientation. Quite remarkably, the largest anisotropy is predicted for interfaces between the prototype free-electron materials silver and aluminium for which a massive factor of two difference between (111) and (001) interfaces is found. This result is insensitive to interface disorder. It could be tested experimentally by means of Andreev reflection.

First-principles scattering matrices in magnetoelectronics

Gerrit E. W. Bauer

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Abstract

Metal-based magnetoelectronics utilizes the interaction of the magnetic order parameters in hybrid structures with electric currents for sensor and data storage application. The transport properties of metallic magnetic nanostructures such as spin valves are often dominated by interface scattering, for which the scattering matrix can be computed by first-principles. In diffuse systems spin and charge transport is governed by a trace of the scattering matrix, viz. a 2x2 conductance tensor, for each resistive element such as an interface between a normal metal and a ferromagnet [1]. For heat transport, the energy derivative of the conductance tensor at the Fermi surface is required as well. In this talk I will briefly introduce the underlying magnetoelectronic circuit theory and review a number of examples of observables in magnetic nanostructures that are accessible to parameter-free calculations.

[1] A. Brataas, G.E.W. Bauer, P.J. Kelly, Physics Reports 427, 157 − 255 (2006).

First principles description of inelastic transport in atomic and molecular wires

Magnus Paulsson

MIC DTU, Denmark

Abstract

Several research groups currently investigate inelastic effects in electron transport through nano-sized devices. In this work we describe our efforts to combine first principles density functional methods (SIESTA / TranSIESTA) with the non-equilibrium Green's function (NEGF) theory to model the conductance including inelastic effects. For a given system we calculate (i) relaxed geometries, (ii) vibrational frequencies, (iii) electron-phonon couplings, and (iv) the inelastic current-voltage characteristics. To illustrate the theory we provide two examples where comparison to experimental data is possible. We have applied our method on atomic gold wires for which high quality experimental data are available [1]. We study comprehensive series of wire geometries containing 3 to 7 atoms under various electrode separations, thereby elaborating our previous results [2]. We further extract quantitative information from the theory, e.g., conductance changes, frequency shifts with strain, and heating effects of the active vibrational modes. These findings are all in very good agreement with experiments. The vibrational effects in three different hydro-carbon molecules connected to gold electrodes were investigated experimentally by Kushmerick et al. [3]. Our theoretical calculations on all three molecules are in good agreement with their measurements [4] and provide insights into (i) which vibrational modes are responsible for inelastic scattering, (ii) the width of the inelastic electron tunnelling signals, and (iii) the mechanisms of heating and cooling of the vibrational modes induced by the coupling to the charge carriers.

References

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[2] Frederiksen, T.; Brandbyge, M.; Lorente, N.; Jauho, A.-P. Phys. Rev. Lett. 2004, 93, 256601.
[3] Kushmerick, J. et al. Nano Letters 2004, 4, 639.
[4] M. Paulsson, T. Frederiksen, M. Brandbyge, Nano Lett. 6, 258 (2006)

Time-domain ab initio studies of ultrafast excitation dynamics in nanomaterials

Oleg Prezhdo
University of Washington, United States

Abstract

Non-adiabatic molecular dynamics techniques implemented within time-dependent density functional theory are applied to study ultrafast photoinduced processes in dye-sensitized semiconductors, quantum dots (QDs) and carbon nanotubes (CNTs). The interfacial electron injection from molecular chromophores into TiO2 surfaces drives the Gratzel solar cell and exemplifies the molecule-bulk interface common to molecular electronics and photoelectrochemistry. The electron-vibrational and Auger relaxations of photoexcited states in QDs determine the efficiencies of hot carrier accumulation and carrier multiplication in QD solar cells. The electron-phonon scattering in CNTs affects nanotube conductivity and characterizes nanotube potential for use in nanoscale electronic devices. The real-time atomistic simulations provide detailed description of these processes.

References

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2. W. R. Duncan, W. Stier and O. V. Prezhdo “Ab Initio Simulations of Photoinduced Molecule-Semiconductor Electron Transfer” in Book Nanomaterials: Design and Simulation, Vol. 18, P. Balbuena, J. Seminario (Eds.), Elsevier, 2006

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4. H. Kamisaka, S. V. Kilina, K. Yamashita and O. V. Prezhdo, “Ultrafast vibrationally-induced dephasing of electronic excitations in PbSe quantum dots”, Nano Lett., in press

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semiconducting carbon nanotube", Phys. Rev. Lett. 96 187401 (2006)

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Multilayer transport calculations within the CPA including vertex corrections

Karel Carva
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Abstract

Ab initio calculations based on Kubo-Greenwood linear response theory have turned out to be succesfull in predicting spin-dependent transport properties of magnetic multilayers. One of the main remaining problems here is to deal with substitutional disorder, which comes from alloying in layers or from interdiffusion at interfaces. In existing works based on calculations from first principles this was usually solved using the supercell method. An alternative way is to use the coherent potential approximation (CPA). In our calculations we employ the full CPA for transport including vertex corrections, which are neccesary to obtain two-particle properties. This concerns spin-dependent charge conductances as well as spin-mixing conductances. Ballistic and diffusive parts of electron transport are treated on equal footing within this approach.

This technique is implemented within the tight-binding linear muffin-tin orbital (TB-LMTO) method and is used to calculate magnetoresistances and mixing conductances of various metallic based multilayers and examine the role of interface interdiffusion or bulk impurities [1]. It can also be applied to a very promising spintronics material: diluted magnetic semiconductors. We calculate magnetotransport properties of thin (Ga,Mn)As slabs including its dependences on the impurity concentration and layer thickness.

Our results show remarkably good agreement with calculations based on the supercell method and with experiments, while the computational requirements remain modest. The calculations demonstrate the importance of vertex corrections for transport properties calculations of real materials and the ability of the full CPA to evaluate efficiently and correctly transport in layered systems.

References

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Finite element implementation of NEGF for nanostructures

Martti Puska
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Abstract

Computational modeling of electron transport through lithographic nanostructures, structured materials, and even single molecules is an essential subfield in the development of future nanoelectronics. Non-equilibrium Green's function formalism (NEGF) applied within the density-functional theory (DFT) offers a practical first-principles modeling scheme. Its popular implementations are based on expansions using localized functions such as atomic orbitals leading to a matrix presentation. We have provided an alternative approach based on the finite element method [1]. The FEM implementation is done within the weak formulation of the equation defining the Green's function. Our tests and applications range from modeling coherent electron transport through layered systems (e.g. resonant tunneling device) [2] and constrictions in the two-dimensional electron gas [3] treated within the effective mass approximation to the calculation of conductance of thin oxide layers described by non-local pseudopotentials [4].

References

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[4] Havu, P., Havu, V., Puska, M. J., Hakala M. H., Foster, A. S., and Nieminen R. M., First principles electron transport: finite-element implementation for nanostructures, J. Chem. Phys. 124, 8 (2006); Hakala, M.H., Foster, A.S., Gavartin, J.L., Havu, P.,Puska, M.J., and Nieminen, R.M., Interfacial oxide growth in silicon/high-k oxide interfaces: first principles modelling of the Si-HfO2 interface, J. Appl. Phys. 100, 043708 (2006).

Long-time dynamics of the Kohn-Sham system for open molecular junctions

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Abstract

We use non-equilibrium Green's function theory to study the asymptotic time-evolution of a Kohn-Sham (KS) electrode/molecule/electrode system. We show that the steady-state assumption is consistent with a smooth local density of states but not with the existence of bound states. In the former case the steady-current can be expressed in a Landauer-like formula with transmission probabilities for scattering of electrons against the asymptotic KS potential. In the presence of bound states the KS system does not evolve towards a steady regime. The density oscillates with history-dependent amplitudes and, as a consequence, the effective potential of TDDFT oscillates too. Such time dependence might open new conductive channels, an effect which is not accounted for in any steady-state approach and might deserve further investigations.

First-principles scattering matrices for spin-transport

Maciej Zwierzycki

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Abstract

Details are presented of an efficient formalism for calculating transmission and reflection matrices from first principles in layered materials. Within the framework of spin density functional theory and using tight-binding muffin-tin orbitals, scattering matrices are determined by matching the wave-functions at the boundaries between leads which support well-defined scattering states and the scattering region. The calculation scales linearly with the number of principal layers N in the scattering region and as the cube of the number of atoms H in the lateral supercell. For metallic systems for which the required Brillouin zone sampling decreases as H increases, the final scaling goes as H2N. In practice, the efficient basis set allows scattering regions for which H2N $\sim$ 106 to be handled. The method is illustrated for Co/Cu multilayers and single interfaces using large lateral supercells (up to 20 x 20) to model interface disorder. Because the scattering states are explicitly found, "channel decomposition" of the interface scattering for clean and disordered interfaces can be performed. Other applications of the method include the anisotropy of interface scattering, spin-transfer and spin-injection.

Conductance, surface traps and passivation in doped silicon nanowires

Marivi Fernandez-Serra

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Abstract

By means of ab initio total energy and conductance calculations within the Landauer Formalism we investigate the structural, electronic and transport properties of doped silicon nanowires (SiNWs). We find that impurities always segregate at the surface of unpassivated wires, reducing dramatically the conductance of the surface states. Upon passivation, we show that for wires as large as a few nanometers in diameter, a large proportion of dopants will be trapped and electrically neutralized at surface dangling bond defects, significantly reducing the density of carriers. Impurities located in the core of the wire induce a strong resonant backscattering at the impurity bound state energies. Surface dangling bond defects have hardly any direct effect on conductance. Upon surface trapping, impurities become transparent to transport, as they are both electrically inactive and do not induce any resonant backscattering.

References

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First-principles calculation for electron conduction properties using real-space finite-

different method

Tomoya Ono

Oasaka University, Japan

Abstract

Within the last several years, a large number of experimental and theoretical studies of ballistic electron conduction through nanoscale junctions such as quantized conductance or ballistic transport have been carried out. Future research on conduction properties can be expected to lead to new discoveries of nanoscience and novel fabrications of electronic devices. So far, we have developed the first-principles calculation method with the incorporation of the overbridging boundary matching formalism and the real-space finite difference approach [1] to elucidate the relationship between geometrical structures and electron conduction properties in which nanostructures are suspended between two semi-infinite electrodes. We will present our computational procedure and the results of the following simulations.

(1) Helical gold nanowire [2] Multishell helical gold nanowires (HGNs) suspended between semi-infinite electrodes are found to exhibit peculiar electron-conduction properties. Our results that the numbers of conduction channels in the HGNs and their conductances are smaller than those expected from a single-atom row nanowire verify the recent experiment. In addition, we obtained a more striking result that, in the cases of thin HGNs, distinct magnetic fields are induced by the electronic current helically flowing around the shells. This finding indicates that the HGNs can be good candidates for nanometer-scale solenoids.

(2) C60 bridge [3] Transport properties of C60 molecules suspended between semi-infinite gold electrodes were examined. Our results indicate that the conductance of the C60 dimer is ~ 0.1 G0 owing to the scattering of incident electrons at the junction between the molecules, whereas that of the C60 monomer is ~ 1 G0. By encapsulating lithium atoms in their cages, the dimer exhibits good conductivity. The energy of the unoccupied molecular orbitals at the junction shifts down to the Fermi level, and as a consequence, the conductance of the Li@C60 dimer significantly increases. To explore the doping mechanism of the C60 bridges, we also compared the energy band structures of the infinite C60, Li@C60, and lithium chains and found that the Li@C60 chain is a conductor due to the electron transfer from the lithium atom to the fullerene, while the other chains are insulators.

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First-principles calculations of spin-dependent tunneling and spin-disorder resistivity

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Abstract

I will present the results of first-principles calculations for different magnetic tunnel junctions focusing on such features as the role of atomic and electronic structure at the interfaces, defects in the insulating barrier, as well as spin-orbit coupling. Spin-disorder resistivity in transition-metal ferromagnets will also be considered.

Our studies suggest that the spin polarization is largely determined by the properties of the ferromagnet/insulator interfaces [1]. A simple tight-binding model demonstrates that the existence of interface states and their contribution to the tunneling current depend on the degree of hybridization between the orbitals on metal and insulator atoms. The decisive role of the interfaces is further supported by studies of spin-dependent tunneling within realistic first-principles models of Co/Al2O3/Co, Fe/MgO/Fe, and Co/SrTiO3/Co tunnel junctions. Variations in the atomic potentials and bonding near the interfaces have a profound effect resulting in the formation of interface resonant states, which dramatically affect the spin-dependent tunneling properties.

We also study the influence of spin-orbit coupling on the electronic structure and spin-dependent tunneling from the Fe(001) surface [2]. Despite its small value, the spin-orbit coupling is responsible for qualitative changes in the properties of surface states and resonances. First, spin-orbit coupling may transform surface states into surface resonances by mixing them to otherwise orthogonal bulk states. Second, due to the Rashba effect, surface resonances shift when the magnetization direction is changed. These shifts may induce large changes in the tunneling conductance. In a tunnel junction with a non-magnetic second electrode, this tunneling anisotropic magnetoresistance may be utilized as an alternative device architecture. Third, spin-orbit interaction induces spin-mixing of the electronic states and opens the spin-flip conduction channels. The spin-flip currents are usually small, but in certain cases they may acquire resonant features and rival the spin-conserving currents. The conditions required for this effect are elucidated using a simple model.

In addition, I will report our results on spin-disorder resistivity of Fe and Ni obtained using the noncollinear density functional theory [3]. The Landauer conductance is averaged over random disorder configurations and fitted to Ohm's law. The distribution function is approximated by the mean-field theory. The dependence of spin-disorder resistivity on magnetization in Fe is found to be in excellent agreement with the results for the isotropic s-d model. In the fully disordered state, spin-disorder resistivity for Fe is close to experiment, while for fcc Ni it exceeds the experimental value by a factor of 2.3. This result indicates strong magnetic short-range order in Ni at the Curie temperature.

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High TMR ratio in Fe/MgO/Fe junctions with even one atomic Fe layer

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Abstract

Recent experiments [1] based on epitaxially grown Fe/MgO/Fe samples shed light on the microscopic origin of tunneling magnetoresistance (TMR). First of all, the obtained TMR ratios exceeded the predictions by Julliere's model. Second, the bias voltage characteristic shows features which could be related to the electronic structure of the system.

The aim of this contribution is to demonstrate how the interface structure, the barrier thickness, and especially the finite thickness of the Fe electrode layers influence the TMR ratio and the corresponding voltage dependencies. Three junction geometries are considered with ideal interfaces and with a mixed Fe oxide layer experimentally found at the Fe/MgO interface. A screened Korringa-Kohn-Rostoker (KKR) method based on density-functional theory was applied to calculate the electronic and magnetic structure of the different junctions selfconsistently. The Landauer conductance of planar junctions was calculated using the Baranger- Stone scheme by means of Green's functions. The bias dependence of the tunneling conductance and the magnetoresistance were computed in the limit of coherent transport. Positive and negative TMR ratios are obtained as a function of interface structure and even a sign reversal of TMR as a function of bias was found [2]. The results demonstrate that the current voltage characteristic is dominated by the interface electronic structure rather independent on the barrier thickness. Finally, junctions with finite Fe layer thicknes and non-magnetic leads will be discussed. It will be shown that the leads have just to provide states of Delta_1 symmetry which tunnel most efficiently across the barrier and the spin-filter effect is generated by even one monolayer of Fe [3].

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Classical Nuclear Motion in Quantum Transport

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Abstract

A quantum-classical mixed scheme is presented to study nuclear dynamics in time-dependent quantum transport. The nuclei are treated in the Ehrenfest approximation. Two model systems are discussed to illustrate the method. The results show how electron-nuclei interactions may induce dynamical Peierls distortions in short wires, and how the behavior of the wires can change

from conducting to insulating. We also provide an example of current-induced molecular desorption and suggest that AC biases could provide a way to tailor electromigration. The results show the importance of non-adiabatic effects for transient phenomena in nanodevices.

Ferroelectric and Multiferroic Tunnel Junctions

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Abstract

So far almost all the existing tunnel junctions have been based on non-polar dielectrics. An interesting possibility to extend the functionality of tunnel junctions is to use a ferroelectric insulator as a barrier to make a ferroelectric tunnel junction (FTJ) [1]. FTJs offer exciting prospects for device applications. In particular, the electric-field-induced polarization reversal in a ferroelectric barrier may have a profound effect on the conductance of a FTJ. One of the mechanisms is the incomplete screening of polarization charges which makes the depolarization field and hence the potential profile seen by transport electrons different for the opposite polarization orientations. In addition, the polarization switching changes positions of ions near the interfaces which affect the atomic orbital hybridizations at the interface and electronic properties of the barrier and hence alter the transmission probability. Functional properties of a FTJ can be extended by replacing normal metal electrodes by ferromagnets which makes the junction multiferroic. In such a multiferroic tunnel junction (MFTJ), where a thin ferroelectric film is used as a barrier, spin-dependent tunneling may be controlled by reversing the electric polarization of the ferroelectric. In addition, by changing the electric polarization of the barrier one can influence the interface magnetic moment and the interface magnetic anisotropy. Thus, such a MFTJ which combines ferromagnetic electrodes and a ferroelectric barrier provides a new degree of freedom in magnetoelectronic devices. This talk will address the physics of FTJs and MTJs based on our recent model and first-principles calculations.

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Strong correlation and order-N in quantum transport: the Smeagol project

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Abstract

Density functional theory has revolutionarized our way to do materials science and it is now a fundamental asset for research in Physics, Chemistry, Biology and Nanoscience. This is mainly due to a combination of conceptual simplicity, rigorous theoretical foundation and efficient numerical algorithms. The Smeagol [1,2] project (www.smeagol.tcd.ie) has the ambitious goal of setting the same revolution in the field of ab initio quantum transport.

Smeagol, in its present form, calculates the I-V characteristics of nanoscale two-probe devices

from first principles. It combines a non-equilibrium transport algorithm capable of evaluating the effects of a steady state current on the electronic structure of the device with density functional theory implemented on a localized atomic orbital basis set. Smeagol is constructed with three main goals in mind. First it must be accurate. For this reason exchange and correlation potentials including strong correlation corrections (LDA+U or LDA+SIC) have been implemented and demonstrated effective for the transport. Secondly, it must be able to scale, and therefore capable of accessing massive parallel machines. Finally it must be reasonably user friendly to serve a large community.

In this talk I will review the basic ideas behind the Smeagol project and present some of our results. In particular I will tackle two problems. First I will discuss transport through simple molecules attached to Au leads, and demonstrate that a computational undemanding method for self-interaction correction can yield results in good agreement with experiments. Then I will tackle the problem of the conductivity of DNA and demonstrate that simulations of devices exceeding several thousands atoms are in the reach of Smeagol's computational capabilities.

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Electronic transport through Wannier functions: from molecular to solid state systems

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Abstract

The current limits of semiconductor electronics and the challenges for future developments involve the continuous shrinking of the physical dimensions of the devices and the attainment of higher speeds. The drive to produce smaller devices has led the current research towards a new form of electronics, in which nanoscale objects and molecular devices replace the transistors of today's silicon technology. Because the electronic operation of a device strongly relies on transport properties, a deep understanding of this new area, along with the development of dedicated experimental and theoretical tools, is of central interest for this scientific area, thus supporting the large effort set up in this direction. From a theoretical point of view the study of electronic and transport properties of molecular systems at the nanoscale requires the review of standard concepts such as bonding, metallicity or magnetism at low dimensionality and in low coordination regimes.

We adopted an ab initio theoretical approach based on density functional theory implemented using plane-waves and ultrasoft pseudopotentials. The transport properties of prototypical lead/molecule/lead systems are calculated by means of an original approach [1] (WanT code [2]) through the use of maximally-localized Wannier functions,[3] within the well established Landauer theory. The method, originally devoted to the study of spinless coherent transport, has been recently extended in order to address the effects of spin-polarization as well as the electron-electron interaction [4]. These kind of effects have been recently demonstrated to play a crucial role in spintronic and nanodevice applications. Finally, we considered the extension of our scheme to the case of massive 3D systems, such as multilayers and interfaces, in which the lateral interactions (typically underestimated in standard approaches) may drastically affect the overall transport properties of the system.[5]

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Hydrodynamic approach to transport in nano-systems

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Abstract

The usual approaches to study transport in nanoscale systems, while able to predict many interesting properties, say nothing about the nature of the electron collective state and its time evolution. Nowadays numerical techniques allow for the first time the study of the full dynamics of a many-particle system starting from first principles. However, in order to implement these techniques to nanoscale systems a deep understanding of the underlying physics is necessary. For these systems we recently showed that one can effectively describe the dynamics of the density and current density by means of a set of equations that are formally identical to the Navier-Stokes equations of fluid dynamics [1]. This result opens up the possibility to simulate the dynamics of the many-body quantum system by solving the equations of motion of an equivalent classical fluid, when the due changes of scale are performed [2, 3]. As a bonus, this theory allows us to transfer a plethora of physical results of classical fluid dynamics to the quantum case [1]. In this talk I will discuss the approximations at the heart of our approach, and some applications to transport and related phenomena like turbulence of the electron liquid [1,2] and local electron heating in nanojunctions [4].

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Ab-initio TB-LMTO method for nonequilibrium electron transport in nanosystems

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Abstract

We present an ab initio method for calculation of the electron structure and electronic transport of nanoscale systems coupled to electrodes with applied voltage bias. The method is based on the local density approximation of density functional theory and implemented in the framework of the tight-binding linear muffin-tin orbital (TB-LMTO) approach in its atomic sphere approximation. A fully atomistic description of the electrodes and the nanosystem is used, and the self-consistent charge and electrostatic potential for the system under applied bias is calculated using the nonequilibrium Green's function (NEGF) approach. General expressions for the lesser Green's function and transmission coefficient obtained within NEGF theory are rewritten using auxiliary Green's functions that are defined by the inverse of the short-ranged structural constants. This reformulation of the theory with auxiliary Green's functions allows the use of very effective and well developed tight-binding techniques. The method is applied to four systems: a single benzene di-thiol molecule coupled to (111) gold electrodes, a single gold atom coupled to (100) gold electrodes, a single platinum atom coupled to (100) platinum electrodes, and pi-stacked polythiophene multilayers coupled to (111) gold electrodes.

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Impurities in atomically-thin metallic nanowires

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Abstract

Metalic nanowires have attracted a great deal of attention lately, since they show very interesting properties from a basic science viewpoint, as well as great potential in applied fields such as nanoelectronics [1]. In this work we have investigated, trough ab initio calculations [2], the effects of the presence of Oxygen and Carbon atoms in atomically thin gold and silver nanowires [3,4]. We have considered several structural configurations, and have also obtained transport properties, based on the coupling of Non-Equilibrium Green's Functions and Density Functional Theory formalisms. The aim of the simulations is to compare these theoretical predictions to recently published experimental results [5].

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Open boundaries and the CEID formalism

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Abstract

Correlated electron-ion dynamics (CEID) is an extension of molecular dynamics that allows us to introduce in a correct manner the exchange of energy between electrons and ions. The formalism is based on a systematic approximation: small amplitude moment expansion. In this talk, we will present two time-dependent methods based on single-particle electron density matrices that allow the electronic and ionic degrees of freedom to be modelled within the CEID formalism in the presence of open boundaries. We will describe a practical implementation using tight binding, and use it to investigate steady-state conduction through a single-atom device, presenting results on inelastic scattering features in I-V curves.

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Sources, sinks and correlations in electron transport

Giorgos Fagas

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Abstract

Modelling quantum transport from first-principles has proven to be a challenging task; debate continues as to the proper theoretical approach for treating electron currents across metal-molecule-metal junctions. Here, we will present an alternative physical scheme that enables to define reservoir boundary conditions at the many-body level, and its implementation leading to the calculation of IV curves for molecular scale systems [1]. We will also discuss how to apply approximate reflection-free absorbing boundary conditions to correlated electron transport cal-

culations [2]. The explicit treatment of electron-electron interactions allows us to investigate the extent of correlations beyond the single-particle picture as we gradually remove approximations towards the higher-level of calculations. Applying the method to tunnelling currents observed in molecular junctions, we identify conditions for defining a "best" independent particle model [3]. Maximisation of the overlap of a Slater determinant composed of single particle states to the many-body current-carrying state is more important than energy minimization for defining single particle approximations in a system with open boundary conditions. Hence, the most suitable single particle effective potential is not one commonly in use by electronic structure methods, such as the Hartree-Fock or Kohn-Sham approximations.

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Influence of disorder on tunnel magnetoresistance

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Abstract

In spite of recent success in observing large values of tunnelling magnetoresistance (TMR) in epitaxial FeCo—MgO—FeCo magnetic tunnel junctions (MTJ's), the values reported are still two orders of magnitude lower than those predicted by first-principles transport calculations for ideal, defect-free MTJ's. In this talk, we present results of a systematic study of the influence of roughness and leads disorder on TMR in a FeCo—vacuum—FeCo model system. Our study is based upon a tight-binding muffin-tin orbital (TB-MTO) implementation of the Landauer-B"uttiker scattering theoretical formulation of transport. Disorder is included in the transport calculation using large lateral supercells.

In the case of ideal, perfectly ordered systems, we find values of TMR comparable in size to those predicted by others in which the mechanism responsible is the very effective transmission through resonant states close to the Fermi level for the minority spin channel. Roughness is found to quench these resonances leading to a drastic reduction of TMR to values comparable to those seen in experiment. As might be expected, the TMR is found to be inversely proportional to the amount of roughness. By performing the calculations for a wide range of concentrations of roughness, we provide a first indication of the deviation from order required to explain current experimental observations. Leads disorder is found to quench the TMR but less strongly than roughness.

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Correlated Electron-Ion Dynamics in molecular systems

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Abstract

Correlated Electron-Ion Dynamics (CEID) has been applied successfully to Joule heating in nanowires. For these systems there are many energy surfaces that have similar shape, but which are weakly coupled. In this limit there is a steady but essentially continuous transfer of energy between the electrons and nuclei, and the main effect on the nuclear system is a broadening of the wavepackets. Furthermore, electron-electron correlation is weak, and a single particle picture is appropriate. In conjugated polymers the picture is different. First, electron-electron correlations are important. This is most easily handled by constructing explicit energy surfaces that can be computed using accurate quantum chemistry techniques. Second, there can be abrupt changes in the structure of the nuclear wavepackets at crossings between surfaces. This can result in complex structures which require high order expansions to describe. We have reformulated CEID in terms of the Wigner function, which we then expand in terms of oscillator wavefunctions. We show that it is able to describe transitions between pairs of parabolic energy surfaces with crossings. Finally, some preliminary results for excited state dynamics in polyacetylene strands described using the SSH model and Ehrenfest dynamics are presented.

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Korringa-Kohn-Rostoker Green-function formalism for ballistic transport

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Abstract

We present a method for the calculation of ballistic transport from first principles. The multiple scattering screened Korringa-Kohn-Rostoker (KKR) method is combined with a Green-function formulation of the Landauer approach for the ballistic transport [1]. We obtain an efficient O(N) algorithm for the calculation of ballistic conductance through a scattering region connected to semi-infinite crystalline leads. The formalism of Baranger and Stone [2] is generalized to the case of Bloch wave boundary conditions; we discuss relevant properties of the S matrix. We consider the implications on the application of the formalism in conjunction with a cellular multiple scattering description of the electronic structure, and demonstrate the convergence properties concerning the angular momentum expansions.

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Avoiding self-repulsion in density functional description

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Abstract

We examine the effects of self-repulsion on the predictions of charge distribution in biased molecular junctions by the local density functional theory methods. This is done using a functional with explicit long-range exchange term effects [R. Baer, D. Neuhauser, Phys. Rev. Lett. 94 (2005) 043002]. We discuss in detail the new density functional, pointing out some of the remaining difficulties in the theory. We find that in weakly coupled junctions (the typical molecular electronics case) local-density functionals fail to describe correctly the charge distribution in the intermediate bias regime.

Applications of the Smeagol code to atomic and molecular junctions

Jaime Ferrer
Universidad de Oviedo, Spain

Abstract

A brief overview of the spin- and molecular electronics code SMEAGOL will be presented. The main body of the talk will be devoted to present some of our results on electrical and spin transport through atomic and molecular chains, and on single-molecule junctions.

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Nanoelectronics with ALACANT: Fundamentals and applications

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Abstract

ALACANT (ALicante Ab initio Computation Applied to Nanotransport) [1] was born in 2000 aiming at an efficient implementation of the non-equilibrium Green function formalism for electronic transport using first principles. While the electrodes far away from the core of the device are modeled by a parametrized Bethe lattice, the core is described by density functional theory (DFT) and gaussian basis sets, as implemented in GAUSSIAN.

The initial belief that the use of DFT would guarantee a quantitative comparison between theory and experiments in nanoelectronics has been substituted by a more realistic view where even the simplest cases turn out to be challenging. As an example of this I will present results for Ni nanocontacts [2] to show that even these simple systems already challenge our understanding and modelling capabilities.

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The TranSIESTA/ATK method

Jeremy Taylor

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Abstract

In this talk, we will review the concepts and implementation of an NEGF-DFT method for quantum transport based on a localized basis set. Selected applications of the method will also be presented.

All-electron calculations of electronic transport: applications to magnetic tunnel junctions

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Abstract

In recent years one witnessed an increasing quest for calculations of electronic transport properties from an ab initio description of the electronic structure in order to provide an understanding of the complex physics of spin-dependent transport in planar tunneljunctions. The interplay between the electronic structure, the details of the atomic arrangement and the magnetism in these planar junctions make the description of electronic tunneling in realistic tunneljunctions a very challenging task.

Most codes used in this field employ a localized basis which supports a partitioning of the Hamiltonian into separate contributions arising from the leads and the interface region. Motivated to describe electronic transport in the context of an all-electron full-potential scheme, we implemented the Green-function embedding formalism within the framework of the fullpotential linearized augmented plane wave (FLAPW) method [1]. This approach allows the calculation of the embedded Green function of the finite scattering region with the correct boundary conditions of attached semi-infinite leads, which appear as additional non-local potentials in the transport calculations.

We will present results for two prominent systems: (i) Fe/MgO/Fe based tunneljunctions [3], which developed to the most important magnetic tunneljunction in the field of TMR devices [4] and (ii) a SrRuO3/SrTiO3/SrRuO3 three-layer junction, where SrRuO3 is a ferromagnetic metal and SrTiO3 forms an insulating barrier. We discuss the role of the interface structure and chemistry on the spin-polarization of the electronic transmission in these systems.

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The flow of molecular orbitals driven by gate or bias voltage in transport calculations based on density functional theory

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Abstract

The charge transport through single molecules is controlled by the shape and energy of individual molecular orbitals. Both of these parameters are modified, they ”flow”, if a bias voltage or an external gate voltage is applied. This orbital flow can have a pronounced impact on the measured I-V characteristics. In our presentation, we will report about two case studies benzene (BDT) and bipyridine. It will be demonstrated, that in particular in the second case the DFT-based level flow is seriously impaired by artifacts of LDA and GGA functionals. An attempt will be made, to disentangle these artefacts from the real physics.

Spin-transport calculations in magnetic materials with presence of spin-orbit coupling and disorder

Anton Starikov
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The physics and chemistry of molecular devices for moletronics and for the post CMOS era

Jorge Seminario
Texas A&M University, United States

Abstract

We report field induced conformational changes in bimetallic oligoaniline junctions [1]. Three types of non-planar conformations are found for a neutral isolated oligoaniline molecule as well as for an oligoaniline with Au and Pd atoms attached at its ends. Each type of conformation has several conformers of nearly equal energies. An applied external voltage can be used to switch between conformations, producing in the process a sharp decrease of their energies. These bias voltage-induced conformational changes are a potential switching mechanism for two terminal molecular devices at the nanoscale domain. They cause the conductivity of the molecule to alternate between high and low states, compensating for the behavior of typical three-terminal devices, needed for the development of a gate-less electronics. Alternative scenarios for molecular electronics based on molecular potentials and vibrations will be also presented [2, 3].

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Quantum Transport in Post-CMOS Molecular Materials & Devices :

Stefan Roche
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Abstract

The downsizing limits of conventional CMOS technologies are requiring the development of advanced computational schemes and methodologies to support material and device engineering strategies. Bottom-up driven PostCMOS-molecular based nanodevices are envisioned as potential alternatives to circumvent CMOS limitations, including device performances, innovative architectures and enhanced functionalities (interconnects, molecular memories, bio-sensing capability, NEMS, etc..). Carbon nanotubes and semiconducting nanowires offer unique low-dimensional materials for improved quantum transport (including charge, spin, phonon and excitons), whose precise scaling properties need however to be ascertained, to allow these material to develop future mainstream technologies. Indeed, despite their spectacular physical properties, a large number of issues remain to be solved to clarify the intrinsic roadmap of POST-CMOS molecular nanodevices.

In this talk, I will discuss several topics concerning quantum transport in DNA, disordered carbon nanotubes or semiconducting nanowires, outlining novel properties and current directions of challenges.

The importance of hybrid methodology combining state of the art ab-initio calculations to sophisticated effective tight-binding models will be presented, and illustrations will be given in relation with the issues of charge transfer in biomolecules, quantum transport in complex (doped, functionalized nanotubes and wires) for systems in which mesoscopic physics dominate.

The complexity of charge transport in DNA will be first overwieved, and the relevance of effective models and ab initio methods briefly put in perspective. The basics of transport in chemically doped carbon nanotubes will be presented with a characterization of basic scaling laws of elastic mean free paths and localization lengths in the coherent regime. The effect of surface roughness will be also addressed in silicon semiconducting nanowires.

Finally, the effect of electron-phonon coupling on quantum transport considering low energy acoustic and weak localization regimes as well as high energy optic modes and current saturation in the high bias voltage regime.

Challenges ahead will be outlined.

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Poster List

Non-local self-energy operators in quantum transport calculations

Hector Mera
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Abstract

We illustrate the effect that the non-locality range of the electron-electron self-energy operator has in the calculated conductances of simple atomic chains. By considering a simple non-local and energy independent self-energy model based on available GW data for the homogeneous electron gas we show that including non-local exchange-correlation effects the homo-lumo gap increases and as a consequence the conductance of the chains decreases with respect to the LDA conductance.

Fermi level alignment in molecular nanojunctions and its relation to charge transfer

Robert Stadler
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Abstract

The alignment of the Fermi level of a metal electrode within the gap of the highest occupied (HOMO) and lowest unoccupied orbital (LUMO) of a molecule is a key quantity in molecular electronics, which can vary the electron transparency of a single molecule junction by orders of magnitude. We present a quantitative analysis of the relation between this level alignment (which can be estimated from charging free molecules) and charge transfer for bipyridine and biphenyl dithiolate (BPDT) molecules attached to gold leads based on density functional theory calculations. For both systems the charge distribution is defined by a balance between Pauli repulsion with subsequent electrostatic screening and the filling of the LUMO, where bipyridine loses electrons to the leads and BPDT gains electrons. As a direct consequence the Fermi level of the metal is found close to the LUMO for bipyridine and close to the HOMO for BPDT. We also comment on the dependence of the level aligment on interface structure and relate our findings to quantum-chemical concepts such as electronegativity.

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Electron transport in a Pt-CO-Pt contact

Mikkel Strange
Technical university of Denmark, physics, Denmark

Abstract

We have performed first principles calculations, for the mechanics and the electrical properties of a Pt nanocontact with a single CO molecule absorbed [1]. We identify a tilted-bridge configuration for the Pt-CO-Pt structure which is stable and has a conductance close to 0.5G0 (G0=2eˆ 2/h), and we propose that this structure is responsible for an observed peak at 0.5G0 in the conductance histogram for Pt exposed to a CO gas [2]. We explain the main features of transmission function for the Pt-CO-Pt, and show that the conductance is largely determined by a local d-band effect at the Pt apex atom.

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Electron Transport with Coupling to Molecular Vibrations

Iben Sig Kristensen
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Abstract

Recently it has become possible to study the electron transport through individual molecules using break junction techniques. One particularly interesting system which has been studied in Leiden (Holland) [1] is the platinum break junction in a dilute gas of hydrogen molecules. When hydrogen is admitted to the chamber a peak around 1 G0 is appearing in the conductance histogram indicating a particular stable configuration. By comparing experimental and theoretical data it has been established that this peak corresponds to a geometry with a hydrogen molecule bridging the platinum electrodes [2].

By using point contact spectroscopy it is possible to obtain additional information about the junction, namely the differential conductance as a function of bias voltage. It shows a decrease at characteristic voltages corresponding to molecular vibrational frequencies. A simple explanation for these observed features is that the electrons start to get backscattered whenever a molecular vibration is excited.

In our work we will present atomistic calculations which are aimed at getting a more quantitative description of such vibration phenomena in single molecule junctions. For this purpose we include the electron-phonon coupling in our calculations of the conductance by employing the technique of non-equilibrium Green functions. The Born-Oppenheimer approximation is used for separating the vibrational and electronic degrees of freedom and the Green function is expanded

to second order in the electron-phonon matrix element.

For simulating the hydrogen experiment a simple model system is chosen as two chains of platinum atoms bridged by a single molecule. The electronic structure is calculated using a plane-wave implementation of density functional theory and subsequently a localized basis set is formed by transforming the Kohn-Sham eigenstates into Wannier functions. For our model system we find that including a frustrated translated mode results in a conductance drop of the same order of magnitude as observed experimentally. This can be explained by backscattered electrons in the completely open s-channel. But in contrast to the experiments we find also an increase in the conductance caused by the excitation of a transverse mode. This finding can be explained by symmetry arguments, since these modes can couple to the platinum d-orbitals and thereby open new conductance channels. At this point it is still an open question why the experimental data does not show that feature.

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2.1.2 Report on the Workshop “Multiscale Approaches to Nanomechanics”

CECAM, Lyon (France)

5th-7th February 2007

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Summary

This meeting has focused on the application of computer simulations to the study of the microscopic aspects that determine the mechanical behavior of materials. This includes the structure and interaction of atomic-scale defects involved in macroscopic failure (crack tips, dislocation cores, grain boundaries, etc), mechanical and electronic transport properties of nanocontacts, and the interaction between nanoasperities (tips) and surfaces which is behind both the operation of scanning probes and the tribological contact between two materials. All these problems share an essentially multi-scale nature that requires a combined treatment of the different length (or time) scales: e.g. the breaking and formation of atomic bonds are dynamically coupled by long-range interactions (elasticity) to the macroscopic boundary conditions (deformation, load) imposed.

Nanomechanics describes the land where scanning probe experiments at the atomic and nanometer scale, the characterization of nanomaterials (e.g. nanotubes, nanocrystals and biomolecules) and computer simulations are currently meeting. This recently-born field spans both the methodological developments in the theoretical description of the different scales (from first-principles to continuum approaches) and the detailed experimental characterization achieved in the last few years, that provides a natural testing ground for those theoretical methodologies designed to bridge the length and time scales.

Following this perspective, the workshop has gathered 55 participants, including 25 invited speakers and session chairs, working in a broad range of problems and scientific disciplines. The event attracted a significant attention and 30 regular participants had to be selected among the 45 applications received in order to accommodate the meeting in the CECAM premises. The program was design to convey a balanced view of both the grand challenges in Nanomechanics and particularly promising methodological advancements. The 17 invited contributions (50 minutes, including 15 minutes discussion) were delivered by leading experts that provided an in-depth view of different theoretical and experimental approaches developed to address the mechanical and transport properties of systems of increasing size and complexity.The session chairs played a key complementary role, identifying strengths and weaknesses of the different particular approaches and stirring the discussion. The program included a lively poster session with 21 contributions, where the discussion extended well beyond the allocated time in the first evening of the meeting into the breaks in the following days.

The meeting has clearly shown the fundamental advances on the experimental side, based on the application of scanning probes. These detailed measurements, that challenged our current understanding and provide accurate quantitative data (even at the single defect level) to confront with the simulations, are the driving force for new theoretical developments. Two aspects emerge as key candidates for new approaches in order to bridge the length and time gap: the simulation under realistic conditions of the nucleation and mobility of point an extended defects, and the complex dynamics of the nanoasperities, the nanoscale objects that control the macroscopic properties of the mechanical contact between two materials.

Scientific Content and Discussion:Highlights

The program content and the abstracts of the different contributions can be found below. In the following we highlight some of the relevant ideas presented in the invited talks.

The three talks in the first day of the workshop, in a session chaired by Peter Gumbsch, addressed from both a theoretical and experimental perspective most of the relevant problems in the field. The first contribution, by Sidney Yip, provided a nice overview of how atomistic simulations can be used to study the nucleation of defects in an homogeneous material under a large strain deformation. This general paradigm was illustrated with applications to nanoindentation (discussing the competition between twinning and slip, and how to pass the yield criteria from atomistic to continuum simulations), dislocation loop emission (pointing out the problem of overdriving the system when using MD simulations) and chemomechanics (water attack on quartz). He ended with a particularly challenging technological problem that requires multiscaling in both the space and time scales: understanding the time evolution of the shear modulus in cement. The talk by Erik van der Giessen showed that the limitations of both pure atomistic and continuum methodologies in order to predict the size dependence of plastic deformation can be overcome with the discrete dislocation plasticity (DDP) approach. He described the rules behind DDP simulations, showed their predictive power at size scales of tens of micrometers and smaller, and stressed the increasing importance of interfaces and boundaries (leading to hardening by pile-ups and strain gradients) when the dimensions of the sample are reduced. Finally, Joost Frenken described recent experiments on atomic-scale friction, where surprising regimes beyond the usual stick-slip behaviour have been found. These include superlubricity, and thermolubricity in layered solids, and the puzzling friction properties of water adsorbed on surfaces. Understanding these nanotribology experiments seems to require a detailed quantitative consideration of the mechanical response and the dynamics of the more mobile tip apex and the rest of the mechanical sensor as independent objects, that is beyond our current capabilities. The simple models that they have considered already questioned some of the basic assumptions in tribology regarding the microscopic channels and time scales for dissipation, and the definition of a microscopic friction coefficient. This talk promoted a lively discussion that extended into the poster session that closed the first day of the workshop.

The morning session in the second day, chaired by Alessandro de Vita, showed again the confrontation between the experimental challenges and some of the more sophisticated theoretical approaches. The session started with a presentation by Mike Payne on linear scaling ab initio methods. After discussing common features in most of these methods, (e.g. the expansion of the density matrix in terms of localized orbitals and a kernel, and the use of the idempotency to satisfy the orthogonality conditions), he focused on the ONETEP code, describing two key aspects of this implementation: (i) the use of a minimal basis of non-orthogonal generalized Wannier functions (NGWFs) adapted to the local environment , and (ii) the PSINC basis (real linear combination of plane waves) employed to span the NGWFs. He showed the accuracy and scalability of the method with different applications, including biological systems. Oscar Custance introduced the experimental perspective, presenting recent experiments with the atomic force microscope (AFM) operated in the dynamical mode that illustrated its capability to image, manipulate and even to chemically identifiy single atoms on surfaces. He also discussed the contribution of ab initio DFT calculations to the understanding of the imaging, manipulation and energy dissipation mechanisms at the atomic scale, and pointed out some of the problems, that are still waiting for more powerful ab initio or hybrid approaches. Alex Shluger addressed, from a theoretical perspective, the manipulation of surface atoms using either photons or an AFM. The first part of his contribution showed the need of an embedded cluster approach, where sophisticated quantum chemical methods can be integrated in order to describe light-induced selective desorption in oxide surfaces. Later, he described a virtual AFM method, where atomistic calculations, a Kinetic Montecarlo approach to bridge the time scale and a description of the electronics behind the operation of the microscope are integrated in order to provide a full account of the instrument response during the theoretical manipulation of an oxygen vacancy. Gabor Csanyi closed the morning session with a discussion of hybrid simulation schemes, where an empirical potential and a quantum mechanical model are combined into a single molecular dynamics simulation. He described different methodologies, based on the ”learning-on-the-fly” approach, to correct the potential in the relevant region in order to reproduce accurately the quantum mechanical forces, and discussed applications to brittle fracture (showing that reconstructions at the crack tip can lead to enhanced lattice trapping) and the properties of graphene ribbons.

Different contributions related to energy dissipation and friction were scheduled in the afternoon session, chaired by Ugo Valbusa. In the first talk, Jacqueline Krim presented three different experiments challenging our understanding of friction. She put particular emphasis in the complementarity of measurements taken with the quartz crystal microbalance and scanning probes (like the scanning tunneling microscope), pointing out the limitations of our current theories to describe the asperity contact point melting. Bo Persson was expected to provide the theoretical counterpart, with a discussion of contact mechanics and adhesion, but his talk had to be cancelled due to health problems. Michael Urbahk closed, in part, that gap with a model that linked the dynamics of formation and rupture of individual bonds with macroscopic friction properties. His approach, based on the relation between the equilibrium properties of the system and the mechanical forces measured under non-equilibrium conditions, extends its applicability to other relevant fields like the single-molecule pulling experiments designed to understand, from the unfolding process, the three-dimensional structure of proteins. The session ended with a detailed experimental discussion, by Nicolas Agrait, of the mechanical and transport properties of atomic chains formed in metal nanocontacts. The variation of those properties with the strain (including energy dissipation and inelastic currents related to the emission of single phonons) provided a very stringent test to our prospective multiscale approaches.

The morning session of the third day covered both strategies to bridge the time gap and to simulate and understand the implementation of pressure/load conditions, and was chaired by Giovanni Ciccotti. Laurent Pizzagalli presented the well-known ”nudged elastic band” approach for the determination of transition state energy barriers and discussed its application to the study of dislocation mobility. He focused on the calculation of the Peierls stress, pointing out the advantages and limitations of alternative methods based on either a direct calculation (where boundary conditions are the critical issue) or a Peierls-Nabarro approach based on the determination of the generalized stacking fault surface (problematic when the dislocation cores are narrow as in the case of Si). Eric van den Eijden discussed an alternative approach to the simulation of rare events: the string method. He started with a brief summary of transition state theory (that provides the basis for the method) and presented, with a simple two-dimensional example, the fundamentals of this algorithm to move curves over an energy landscape that is able to identify, in its zero- or finite-temperature versions, the minimum energy or minimum free energy paths. He concluded with a realistic application to the determination of the structure of a polymer chain in solvation. The experimental study of small-scale plasticity was the topic of the contribution by Andrew Minor. He showed how nanoindentation experiments performed inside a transmission electron microscopy provide access to a quantitative determination of the yield stress, through the simultaneous measurement of the imposed forces and the imaging of the induced deformations. These experiments, showing, for example, large yield stresses even in the presence of a large number of defects, challenge our understanding of the mechanical response of nanoscale objects. The session concluded with a theoretical talk by Carla Molteni on the simulation of pressure-induced structural transformations in semiconductor systems. She showed how to implement constant-pressure molecular dynamics simulations in both bulk and nanomaterials and discussed applications to the study of size-dependent properties in semiconductor nanocrystals under pressure.

The meeting ended with an afternoon session, chaired by Karsten Reuter, that illustrated the need of coarse-graining approaches to gain some understanding in complex systems. Alexis Baratoff discussed recent experiments where a small sinusoidal excitation of the cantilever leads to a regime with essentially vanishing friction. This novel regime can be understood with a simple extension of the classical friction models that takes into account the separation of the relevant time scales for the cantilever and the nanotip, the few atoms at the tip apex involved in the atomic-scale stick-slip processes. Berend Smit addressed the challenge of simulating the complexity of biological structures like cell membranes were purely atomistic approaches are not viable. Coarse-graining is the key tool to produce a manageable model that captures the repulsive (size-driven interactions) that control the packing and provides a good description of the phase diagram.

Conclusions and Perspectives

Nanotechnology, as an essentially cross-disciplinary field, still lacks the set of well-established concepts that characterize a mature discipline. This meeting has fulfilled the goal of gathering leading researchers from different communities (ab initio practitioners, molecular dynamics experts, material scientists, nanotribologists,) to share their expertise on the microscopic understanding of the mechanical properties of materials. The broad perspective delivered by the quite different topics covered by the invited speakers, and the lively discussions on particular conceptual or methodological aspects have contributed to the balanced view needed to identify common problems and interests. From this perspective, the meeting has contributed significantly to the definition of the core issues and challenges that should pervade the future development of Nanomechanics.

The main conclusions of the meeting can be summarized as follows:

- Although steady progress has been achieved in some particular aspects, this knowledge has not result in a fundamental, basic understanding of the mechanical response of materials. Some key ingredients have been identified (e.g. role of boundaries, defect mobility, see below) but we still lack a common framework that integrates all of them. The dispersion in methodological approaches and computational codes, devised in most cases for very specific applications, reflects this situation.

- Hybrid modelling, where the different length scales are dynamically coupled in a single simulation, is still a formidable task. Hierarchical multi-scale modelling –based on the optimal tools that we have for the different regimes (quantum mechanical, atomistic, quasi-continuum)– offers a viable alternative for many problems, where information can be extracted from one scale and passed to the next.

- Experiments are bridging the gap from the macroscopic to the nanoscale, providing relevant quantitative information (e.g. the yield stress for nucleation and response of a single defect, tip-sample forces for the diffusion of surface atoms) that can be directly used to validate the simulation approaches.

- The competition between nucleation and mobility of defects, and their interplay with boundaries (grains, interfaces,) and the chemical environment are key unifying microscopic concepts in the understanding of the mechanical response. Our current simulation approaches are still quite limited: they are affected by overdriving (due to the large gradients needed to create or move the defect) that contaminates the dynamical results, and they have severe limitations for considering all these processes at the same time.

- The rich phenomenology found in the mechanical contact between two materials (nanotribology) seems to be dominated by the interplay between the mechanical response and the dynamics of both small scale objects (tip apex, nanoasperities) and the macroscopic mechanical sensor considered as independent objects. The quantitative simulation of the resulting complex dynamics is still a theoretical challenge.

From the state of the art reflected in these conclusions, we should expect future developments in the field to follow these lines:

- Hybrid schemes, linking dynamically the different relevant length scales, are expected to play a key role in the final understanding of basic problems like brittle fracture. These developments will unifying concepts and well-tested, powerful codes that would stir further advancements in the field.
- There is an urgent need for new accurate and well-tested formulations to implement efficiently the elastic (load, pressure,..) boundary conditions and to extract information from atomistic simulations (e.g. yield stresses) into coarse-grained models, like Discrete Dislocation Plasticity and continuum approaches.
- A close collaboration between theory and experiment on well-defined problems (like tip-sample interaction in AFM) will make it possible to go beyond the mutual validation into real understanding.
- More systematic and efficient methods to explore rare events and identify minimum energy paths are needed in order to predict quantitatively the nucleation and mobility of defects. A real breakthrough in this field requires a joint effort of the ab initio and molecular dynamics communities.
- New methodological developments to break the time-scale gap (Accelerated Molecular Dynamics methods and efficient Kinetic MonteCarlo-like schemes) are needed in order to improve our fundamental understanding of nanotribology. The connections already identified between some equilibrium properties of nanoscale systems (easier to study theoretically) with the real non-equilibrium measurements performed in the experiments have to be further substantiated and expanded.

Program

Monday, February 5th

14:00 - 14:50	Registration	
14:50 - 15:00	Ruben Perez & Karsten Reuter	Welcome
		Chair: Peter Gumbsch
15:00 - 15:50	Sidney Yip	Nanoscale Characterizations of Shear Localization in Solids
15:50 - 16:40	Erik Van der Giessen	Discrete Dislocation Plasticity: Bridging a Gap
16:40 - 17:10	Coffee & Discussion	
17:10 - 18:00	Joost Frenken	Experiments on Atomic-Scale Friction: Superlubricity and Other Surprises
18:00 - 19:30	Poster Session & Buffet	

Tuesday, February 6th

		Chair: Alessandro de Vita
9:00 - 9:50	Mike Payne	The Linear Scaling Density Functional Theory Code ONETEP
9:50 - 10:40	Oscar Custance	Dynamic Force Microscopy: Imaging Contrast, Manipulation and Chemical Identification of Individual Atoms
10:40 - 11:20	Coffee & Discussion	
11:20 - 12:10	Alex Shluger	Manipulating Surface Atoms using Photons and AFM
12:10 - 13:00	Gabor Csanyi	Hybrid schemes for Atomistic Modelling
13:00 - 14:30	Lunch	
		Chair: Ugo Valbusa
14:30 - 15:20	Jacqueline Krim	Viewing a Moving Contact: A Scanning Probe and Quartz Crystal Microbalance Study of Sliding Friction and Melting at Single Asperity Contacts
15:20 - 16:10	Bo Persson	Contact Mechanics and Adhesin
16:10 - 16:40	Coffee & Discussion	
16:40 - 17:30	Michael Urbakh	Dynamical Rupture of Molecular Bonds: From Single Molecular Studies to Nanomanipulation and Friction
17:30 - 18:20	Nicolas Agrait	Mechanical Properties and Dynamics of Suspended Atomic Chains
19:30	Conference Dinner	

Wednesday, February 7th

		Chair: Giovanni Ciccotti
9:00 - 9:50	Laurent Pizzagalli	Determination of Dislocation Mobility from Transition States Searching Technique
9:50 - 10:40	Andy Minor	Direct Observation and Measurement of Small-Scale Plasticity Phenomena through in situ TEM Nanoindentation and Compression Tests.
10:40 - 11:20	Coffee & Discussion	
11:20 - 12:10	Eric Van den Eijden	String Method to Find the Pathways of Rare Events.
12:10- 13:00	Carla Molteni	Pressure-Induced Structural Transformations in Semiconductor Systems
13:00 - 14:30	Lunch	
		Chair: Karsten Reuter
14:30 - 15:20	Alexis Baratoff	A Novel Mechanism for the Efficient Reduction of Atomic-Scale Friction
15:20 - 16:10	Berend Smit	Simulating Mesoscopic Models of Biological Membranes
16:10 - 16:30	Closing Remarks	

ABSTRACTS OF INVITED TALKS

Nanoscale Characterizations of Shear Localization in Solids

Ting Zhu[1], Ju Li[2], Shigenobu Ogata[3], Jingpeng Chang[4], Krystyn Van Vliet[5], Subra Suresh[5] and Sidney Yip[4,5,*]

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The phenomenon of defect nucleation in a crystal lattice is fundamental to our understanding of materials strength and deformation. Through atomistic simulations we examine how a dislocation slip or a deformation twin can form as a result of shear localization in response to an

imposed stress field. Three scenarios will be described to illustrate our attempts to formulate dynamical measures of such processes at the nanoscale. In nanoindentation of a single-crystal thin film we show a local stiffness criterion can be developed to account for the displacement bursts associated with dislocation nucleation and multiplication. By subjecting a perfect crystal to affine shear we find the formation of a deformation twin evolves as an instability of a non-linear wave. To model the advancement of a crack front we use reaction pathway sampling to determine the saddle-point configuration, which leads to the bowing out of a dislocation loop in the case of a ductile metal (Cu), and the nucleation and propagation of double kinks in the case of a brittle semiconductor (Si). Scrutiny of these results, based thus far on empirical interatomic potentials, by density functional theory methods would be illuminating.

Discrete Dislocation Plasticity: Bridging a Gap

Erik van der Giessen

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Although much is known about the atomic structure of dislocations, the link to what we observe on larger scales as plastic deformation is still largely elusive. A key reason is the large separation of scales, for which the study of individual dislocations remained in the realm of physics while plasticity was an engineering topic. During the last decade however, the gap between these started to be filled by discrete dislocation plasticity. This is an approach where the atoms are averaged-out and treated as an elastic continuum, while the dislocations are regarded as discrete entities. Discrete dislocation computations are useful in the range of size scales where there are too many dislocations to be treated atomistically but not enough to be averaged-out to continuum plasticity. This transition happens to lie around a micrometer, a length scale that is typical in current MEMS applications. Moreover this is roughly the sizescale at which numerous plasticity phenomena are taking place that exhibit size effects inaccessible by standard continuum theories.

In view of the other sessions in this workshop, I will supplement the exposition of the approach with some examples concerning indentation, contact and friction.

Experiments on Atomic-Scale Friction: Superlubricity and Other Surprises

Joost W.M. Frenken

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This talk will provide a brief summary of Friction-Force Microscopy (FFM) experiments, in which a sharp tip is moved over a flat substrate with atomic-scale precision, while the lateral forces are recorded with a sensitivity down to the low picoNewton regime. Whereas the first measurements in this field have demonstrated a variety of atomic-scale lateral force patterns, related to stick-slip motion of the tip in the periodic, two-dimensional surface of the interaction potential between the tip and the substrate, recent experiments and model calculations are revealing important new ingredients. In particular, I will address lattice mismatch effects that can lead to superb slipperiness (*'superlubricity'*), thermal effects that can dramatically lower friction (*'thermolubricity'*) and multiple-mass-multiple-spring effects that can lead to quite unexpected sliding dynamics [3].

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The Linear Scaling Density Functional Theory Code ONETEP

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University of Cambridge, United Kingdom

ONETEP is a density functional theory code that offers the same accuracy as state of the art plane wave approaches but offers efficient and robust convergence to the electronic groundstate in a computational time that scales linearly with the number of atoms in the system. This code allows first principles calculations to be performed for systems containing thousands of atoms at very modest cost both in terms of computational resources and money. The ability to perform calculations for so many atoms provides much greater flexibility in the choice of quantum region in QM/MM or hybrid simulation schemes. ONETEP allows one to choose the range of the density matrix and this can be used to rigorously assess the errors introduced by truncating the QM region in hybrid simulations.

Dynamic Force Microscopy: Imaging Contrast, Manipulation and Chemical Identification of Individual Atoms

Oscar Custance

Graduate School of Engineering, Osaka University, Japan

Dynamic force microscopy is a particularly promising technique in nanoscience. This scanning probe method makes it possible, for instance, to image both conducting and insulating surfaces with true atomic resolution [1], to manipulate atoms at surfaces even under room temperature conditions [2], or to characterize the chemical composition of a surface at atomic scale [3]. Most of these capabilities are closely related to the nanomechanical properties of the surface under study and the tip-apex probing it, linked though the short-range chemical interaction forces between the tip-surface closest atoms. The ability to quantify very precisely these chemical forces [4-6] makes DFM a suitable and challenging method for the combination of experiments and theoretical approaches on nanomechanics. In this contribution we will present some of the latest mayor achievements in DFM, in which the combination of experiments and first-principles calculations has shown to be particularly useful to understand the complicated processes observed [3, 4-7].

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Manipulating Surface Atoms using Photons and AFM

Alexander Shluger

Department of Physics and Astronomy, University College London, Gower St., London WC1E6BT, UK

I will discuss the results of some of our studies of atomic scale contacts between oxide nanoclusters and surfaces using different levels of multi-scale modelling. First, I will focus on applying an embedded cluster technique to study the structure, electronic properties and photo-induced modification of MgO and CaO powders. A variety of structural features will be considered that can be found on the surface of nanoclusters as well as at interfaces between nanocrystallites buried inside the powder. I will then focus on photo-induced desorption of hyper-thermal O, Mg (Ca) atoms from the MgO and CaO surfaces and will show that the yield, electronic state, and velocity distributions of desorbed atoms can be controlled due to preferential excitation of surface excitons. MgO nanoclusters are also used as model tips for simulating non-contact Atomic Force Microscopy imaging of ionic surfaces and manipulation of surface atoms and adsorbates. In this case combining both different length- and time-scales is important. Our simulations predict that controlled manipulation of a charged surface O vacancy and adsorbed atoms, such as Pd, on the MgO (001) surfaces can be achieved via the reduction of diffusion barriers by the tip electrostatic potential, which facilitates thermal diffusion. Modelling of the full manipulation process involves much slower tip oscillations and even slower response of the AFM electronics.

Hybrid schemes for Atomistic Modelling

Gabor Csanyi

University of Cambridge, United Kingdom

I will present updates on our going efforts in hybrid atomistic modelling, whereby an empirical potential and a quantum mechanical model are combined into a single molecular dynamics simulation. Fundamental limitations of this approach will be discussed, along with several ways of combining the two models. Practical examples include fracture, defect energetics and biomolecular modelling.

Viewing a Moving Contact: A Scanning Probe and Quartz Crystal Microbalance Study of Sliding Friction and Melting at Single Asperity Contacts

J. Krim

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Energy transfer plays an important role in many surface processes such as surface diffusion, vibrational relaxation and sliding friction in adsorbed molecules. The Quartz Crystal Microbalance has in recent years been employed to reveal much fundamental information on the phononic and electronic energy dissipation mechanisms associated with the sliding of atomically thin films along surfaces, a phenomenon closely related to the spreading diffusion of a film on its substrate.[1] While in quantitative agreement with theory and computer simulation, the QCM data have not been cross-referenced to scanning probe measurements of sliding friction and diffusive behavior of atoms along surfaces. We have thus combined a Scannning Tunneling Microscope and QCM to allow direct imaging of films adsorbed on the QCM electrode under both stationary and oscillating conditions.[2] The results of these studies will be described, along with a discussion of whether our current knowledge of the fundamentals of friction is sufficient to enable prediction of asperity contact point melting.

[1] *STM, QCM and the Windshield Wiper Effect: A Joint Theoretical-Experimental Study of Adsorbate Mobility and Lubrication at High Sliding Rates.* M. Abdelmaksoud, S. M. Lee, C. W. Padgett"D. Inving, D.W. Brenner, and J. Krim, Langmuir, in press

[2] *Observation of tribo-induced melting of an asperity contact with STM-QCM,* S. M. Lee, D. L. Irving, C. W. Padgett, D.W. Brenner, and J. Krim, Phys. Rev. Lett, submitted

Contact Mechanics and Adhesion

B.N.J. Persson,

IFF, Research Center Jülich, Germany

Adhesion and friction becomes more important when the lateral size of objects decreases. This is due to the increased surface to volume ratio. At the micro and nanoscale the gravitational interaction is usually negligible compared to the van der Waals interaction and electrostatic interactions, or forces due to the formation of small (nanometer) capillary bridges. Problems related to adhesion and friction (and wear) are the most severe problems to be overcomed in the development of many useful micro or nanoscale mechanical systems, e.g., micromotors. In this presentation I will describe a new theory of contact mechanics for solids with randomly rough surfaces. I consider the elastic contact between solids both without and with adhesion. As an illustration I will discuss in detail biological adhesion systems used for locomotion, and show how Natural selection in some cases has optimized the adhesive systems from the (macroscopic) size of the adhesion pads (typically of order _ 1 mm) to the nanoscale. As a second application of the theory I will briefly describe rubber friction on rough substrates.

Dynamical Rupture of Molecular Bonds: From Single Molecular Studies to Nanomanipulation and Friction

Michael Urbakh

School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel.

Single molecular pulling experiments using atomic-force microscopes or laser tweezers are widely used to probe rare molecular events, such as rupture of molecular bonds and protein unfolding. In order to explore the results of these experiments and to reveal a molecular scale energy landscapes, one has to establish relationships between equilibrium properties of the nanoscale systems and the mechanical forces measured under non-equilibrium conditions. Here we introduce a new approach to describe unbinding processes measured by dynamical force spectroscopy experiments that predicts a distribution of rupture forces, and dependences of mean rupture forces and variance on the pulling velocity. It was shown to reproduce the results of simulations without using adjustable parameters. Our analysis predicts that the mean force at rupture is a nonlinear function of the logarithm of the pulling velocity. We show that understanding unbinding processes on the single-molecule level opens new ways for manipulation of individual molecules at surfaces.

We propose a microscopic model that establishes a relationship between the dynamics of formation and rupture of individual bonds and macroscopic frictional phenomena. In particular, the stick-slip regime of motion is shown to correspond to a cooperative rupture of the bonds.

Mechanical Properties and Dynamics of Suspended Atomic Chains

Nicolás Agraït

Low Temperature Laboratory. Universidad Autónoma de Madrid (Spain)

Freely suspended atomic chains form spontaneously during the final stage of rupture of a metal contact of certain metals (Au, Pt, Ir). These nanostructures are very attractive because being so simple in structure they are amenable to detailed theoretical calculations of structure and transport using state-of-the-art ab initio methods, allowing for direct comparison between experiments and theory. Electronic transport and mechanical properties have been studied experimentally and theoretically in some detail. In this talk I will review the mechanical and vibrational properties of atomic chains and present new recent experimental results on the interatomic interaction dynamics in the chains.

Determination of Dislocation Mobility from Transition States Searching Technique

L. Pizzagalli, P. Beauchamp, A. Pedersen, A. Arnaldson, and H. Jonsson

CNRS, France

Dislocations are extended defects present in almost all materials that govern the mechanical response in the plastic regime. Their properties and behaviors under stress are then important to characterize for a better understanding of mechanical properties of materials. Recently, numerous works have been devoted to core dislocations modeling using first principles methods. This especially concerned stability and structure. For a complete understanding of the plastic properties of materials, quantities related to dislocations mobility (critical stress, kinks formation,...) have to be determined as well. However, due to the technical limitations associated with conventional atomistic methods, less informations are available.

Here, we present the results of first principles and potentials simulations on dislocation mobility in semiconductors, using transition states searching technique such as Nudged Elastic Band. In a first part, we show how this technique can be used to determine the Peierls stress of perfect dislocations in silicon, how pressure would affect this value, and how a dislocation shape changes during its displacement. In a second part, we discuss the mobility of dislocations through kinks formation/migration.

Direct Observation and Measurement of Small-Scale Plasticity Phenomena through *in situ* TEM Nanoindentation and Compression Tests

A. M. Minor

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA

The technique of quantitative *in situ* nanoindentation in a transmission electron microscope (TEM) allows for the simultaneous measurement of the imposed forces and imaging of the initial stages of plasticity in materials. Individual yield events in a material can be directly correlated with the stress required to initiate specific deformation events. This talk will demonstrate this capability from results on the in situ nanoindentation of Al thin films and in situ compression of nanostructured Ni and Al pillars. In the Al thin films we have observed that high stresses are achieved in the Al thin films even in the presence of significant defects. In situ compression experiments on single crystal Ni and Al pillar structures directly demonstrate the phenomenon of source-limited deformation, where plasticity is derived from single or very few active slip systems in samples with sub-micron dimensions. These results will be discussed in terms of current and future computational efforts to model and predict similar deformation phenomena.

String Method for the Study of Rare Events

Eric Van den Eijden

Courant Institute of Mathematical Sciences, New York, USA

The string method is a simple and efficient technique for computing accurately minimum energy paths (MEPs) and minimum free energy paths (MFEPs). I will introduce the theoretical background behind the method, discuss its algorithmic details and illustrate it via examples.

Pressure-Induced Structural Transformation in Semiconductor Systems

Carla Molteni

Kings College London, United Kingdom

Pressure can be used as a tool for inducing structural transformations between distinct crystalline and/or amorphous structures. Polymorfism and polyamorphism phenomena can be studied by means of constant-pressure molecular simulations in both bulk- and nano-materials. In particular semiconductor nano-crystals under pressure exhibit a range of interesting size-dependent properties, which need to be dealt with specific techniques for non-periodic systems. Still constant pressure molecular dynamics simulations for structural phase transformations suffer from shortcomings due to the limited accessible time-scale; while solutions have been proposed for periodic bulk systems, methods for non-periodic systems need to be explored. Results and ideas for cadmium selenide and silicon bulk- and nano-crystals will be presented.

A Novel Mechanism for the Efficient Reduction of Atomic-Scale Friction

S. Maier, A. Socoliuc, A. Baratoff, E. Gnecco, E. Meyer

National Center of Competence in Research (NCCR) on Nanoscale Science, Institute of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The transition from atomic-scale stick-slip to continuous sliding with essentially vanishing friction predicted by the Prandtl-Tomlinson model has clearly been observed for a sharp atomic force microscope tip slowly scanned in contact with a cleaved NaCl crystal in UHV [1]. A similar transition under the same conditions has recently been achieved upon excitation of a flexural mode of the cantilever bearing the tip [2]. In contrast to the previously observed or predicted reduction of friction in the presence of driven oscillations [3], the effect is not associated with a time-average increase of the tip-sample distance.

We consider in detail a dynamic extension of the model introduced earlier [1]. On one hand, the observed dependence of the lateral force along the scan direction implies an oscillating corrugation potential experienced by the tip. On the other hand, the observed low contact stiffness suggests that atomic-scale stick-slip mainly involves elastic energy stored and released by a few atoms around the tip apex. Atomistic support this conjecture. These *a priori* unexpected results lead to a model which accounts well for the new measurements in the presence of perpendicular sinusoidal excitation [2]. In view of the separation of the relevant time scales for the cantilever and the “nanotip”, the observed reduction of friction can be explained in terms of parameters extracted from quasistatic measurements alone. Deviations from adiabatic following cause a residual viscous-like friction which is independent of damping and to a concomitant energy loss. Remarkably, the total loss, including the contribution from the periodic actuation, can be considerably smaller than in the absence of the latter. Simple physically motivated approximations can explain our numerical results

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Simulating Mesoscopic Models of Biological Membranes

Berend Smit, Maddalena Venturoli and Frederic de Meyer

CECAM, Lyon, France

In this presentation a mesoscopic model of a biological membrane is presented. We show that this model can correctly describe the phase behaviour of a phospholipid membrane. We investigated the phase behavior of double-tail lipids, as a function of temperature, headgroup interaction and tail length. At low values of the head-head repulsion parameter the bilayer undergoes with increasing temperature the transitions from the subgel phase via the flat gel phase to the fluid phase. We find that the rippled structure occurs if the headgroups are sufficiently surrounded by water. The anomalous swelling, observed at the transition, is not directly related to the rippled phase, but a consequence of conformational changes of the tails. This model is subsequently used to study the effect of alcohol and transmembrane peptides on the structure of the membrane.

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POSTER LIST and ABSTRACTS

1. Metadynamics simulations of phase transitions in solids
   by **Jörg Behler**, Michele Parrinello

2. An efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer Molecular Dynamics
   by **Thomas Kühne**, Matthias Krack
3. Mechanical testing of nanocrystalline ceramics: massively parallel molecular dynamics simulations
   by **Izabela Szlufarska**, Yifei Mo
4. Modelling strategies for ferritic steels
   by **Maria Samaras**
5. Accurate periodic calculations using large Gaussian basis sets
   by **Matthias Krack**
6. Tribological properties of adsorbed Xe-layers on Cu(111) surface
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   by **Giulio Biddau**, M. Basanta, J. Ortega, R. Pérez, G. Otero, B. Gómez-Lor, J.A. Martín Gago
9. First-principles study of the cubic-SiC(100) - 4x2 surface
   by **Daniel Gonzalez**, D. González , P. Jelínek , J. Ortega
10. Density functional embedding for molecular systems
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11. Enhanced chemical reactivity of gold nanowires
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12. Interstitials in FeCr studied by Density Functional Theory
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13. Hydrogen damage in metals: Constrained molecular dynamics and Monte Carlo simulations of superabundant vacancies
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14. Study of In adsorption on a In-rich 2(2x4) InGaAs surface on GaAs(001)
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17. Computational tools for modeling and simulation of nanoscale systems
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19. Relaxation of semiconductor interfaces by molecular dynamics using enhanced bond order potentials
    by **Kurt Scheerschmidt**, Volker Kuhlmann
20. Multiscale hybrid simulations of brittle fracture
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21. A cohesive zone model for stress corrosion cracking in ceramic polycrystals
    by **Rafael Estevez**, M. Romero de la Osa, C. Olagnon, J. Chevalier, C. Tallaron, L. Vignoud

Metadynamics simulations of phase transitions in solids

Jörg Behler, Michele Parrinello

ETH Zurich, Switzerland

The chemical and physical properties of a solid are determined by its crystal structure, which depends on the temperature and pressure in the system. Often, the experimental determination of the crystal structure is very difficult or even impossible under extreme conditions, which are present e.g. in the interior of the earth and other planets. Therefore, in recent years the theoretical prediction of crystal structures has become a valuable tool to investigate solids under these conditions. The stability of a structure is given by its Gibbs free energy, and the hypersurface of the Gibbs free energy can be systematically mapped by the recently developed metadynamics approach. In this method the Gibbs free energy is represented as a function of the unit cell parameters, which are modified by introducing Gaussian potentials. This requires the calculation of the stress tensor for many different unit cells by molecular dynamics (MD) simulations. If no fast and reliable potentials are available the only way to perform the MD simulations is to use potentials obtained directly from Density-Functional Theory (DFT), which for metadynamics is computationally too demanding even for systems of moderate size. In the present work we develop and employ a new type of Neural Network (NN) potential to represent the high-dimensional DFT potential-energy surface (PES) as a function of all atomic coordinates in the crystal. Tests show that an accurate fit can be obtained that correctly describes all known crystal structures of silicon. This NN potential is applied to metadynamics simulations of pressure-induced phase transitions in bulk silicon. We obtain phase transitions in good agreement with density-functional calculations and experiment.

An Efficient and Accurate Car-Parrinello-like Approach to Born-Oppenheimer Molecular Dynamics

Thomas Kühne, Matthias Krack

ETH Zürich, Switzerland

We present a new method to accelerate density functional theory-based ab-initio molecular dynamics simulations. In the spirit of the Car-Parrinello approach, the method circumvents the need to perform fully self-consistent electronic structure calculations. However, in contrast to the original scheme, large integration time steps can be used. To achieve this, we propagate the electronic degrees of freedom in terms of the contra-covariant density matrix in a nearly time-reversible manner by applying the always stable predictor-corrector method. The corrector consists of a single preconditioned minimization step using the idempotency conserving orbital transformation method. In this way sizable minimization steps can be taken, which guarantees that the propagation is performed within a small skin very close to its instantaneous ground state. Although the applied non-self-consistent energy functional is not variational, the energies thus calculated are a strict upper bound. Deviations from the Born-Oppenheimer surface are small and, more importantly constant, which implies that energy differences are portrayed with great accuracy. In spite of these excellent properties the incomplete energy minimization and the use of a non-symplectic integrator for the electronic degrees of freedom induces a small dissipative drift. Inspired by ideas of Krajewski and Parrinello we show how this can be rigorously corrected using a properly modified Langevin equation, which leads to correct sampling of the Boltzmann distribution. Furthermore the friction term is so small that the dynamics is also properly reproduced. The method works well irrespective of system type and band gap, so it is very efficient even in simulating large metallic systems. We implemented these ideas in the mixed Gaussian Plane Wave (GPW) code Quickstep which is part of the publicly available suite of programs CP2K. Using this code we performed extensive tests on liquid semiconductors showing that the accuracy can be maintained throughout. The gain in efficiency ranges from one to two orders of magintude depending on the system.

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Mechanical testing of nanocrystalline ceramics: massively parallel molecular dynamics simulations

Izabela Szlufarska, Yifei Mo

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Atomistic mechanisms underlying the mechanical response of nanocrystalline ceramic thin films have been studied by multimillion-atom molecular dynamics simulations on parallel computers. The increased volume fraction of highly disordered intergranular films as compared to nanometals manifests itself in new deformation mechanisms. Our nanoindentation studies of nanocrystalline silicon carbide provide a scenario for the interplay between grain rotation, corporate grain motion, sliding at grain boundaries and integranular deformation to produce a rich and unique load-displacement response. We predict a crossover from continuous corporate grain response to discrete inter-grain plasticity at a critical depth that is a fraction of the grain size. We have also studied simulated the tensile and shear testing and described changes in the mechanical response resulting from the reduction of a grain size. Understanding of the fundamental phenomena that govern mechanical properties is crucial for design and fabrication of nanocrystalline materials with enhanced mechanical properties.

Modelling Strategies for Ferritic steels

Maria Samaras

Paul Scherrer Institiute, Switzerland

The safe and reliable performance of fusion and fission plants is dependent on the choice of suitable materials and assessment of long-term materials. These materials are degraded by their exposure to high temperatures, irradiation and a corrosive environment, therefore it is necessary to address the issue of long term damage evolution of materials under service exposure in advanced plants. The life-time assessments of these materials requires an understanding of the related physical phenomena on a range of scales from the microscopic level of single defect damage effects all the way up to macroscopic effects. Therefore it is necessary to have an understanding of the mechanisms at play at many different time and length scales. Computer modelling is expected will complement experimental work to enhance and speed up the assessments of the expected life-time of materials subjected to reactor conditions with the formulation of credible predictive computational models. These models must be developed with the verification of experiment, to accurately describe materials phenomena and to allow for extrapolation to longer time frames. In this poster the multiscale modelling strategies undertaken to study ferritic steels are presented. Within this frame work the influence of magnetism on the ferritic system and experimental validation of magnetic ab initio calculations using XMCD and XAFS are presented

Accurate Periodic Calculations Using Large Gaussian Basis Sets

Matthias Krack

Computational Science, ETH Zurich, via G. Buffi 13, 6900 Lugano, Switzerland

Condensed phase calculations using Gaussian basis sets for liquid and crystalline systems are presented. The calculation were performed with the QUICKSTEP code [1, 2]. QUICKSTEP is an implementation of the Gaussian and plane waves (GPW) method [3] based on the Kohn-Sham formulation of density functional theory. The hybrid scheme employed by QUICKSTEP uses a mixed basis set approach combining Gaussian functions and plane waves in order to exploit the advantages of both basis set types. Gaussian basis sets and pseudo potentials optimized for the use with QUICKSTEP are presented to show its accuracy [4]. The computational efficiency of QUICKSTEP allows to use large Gaussian basis sets including functions of high angular momentum and accurate pseudo potentials for systems up to several thousand atoms. The results of benchmark runs for water are presented to show the efficiency and scalability of QUICKSTEP. Moreover, the Gaussian augmented plane waves (GAPW) scheme [5] allows to perform all-electron calculations [6, 7] or to deal with very hard (i.e. accurate) pseudo potentials which are e.g. mandatory for systems containing first-row transition metals. Results of periodic all-electron and pseudo potential calculations for bulk pyrite (FeS2) are compared with other methods.

The QUICKSTEP code is part of the freely available program package CP2K (http://cp2k.berlios.de).

Acknowledgments

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Tribological properties of adsorbed Xe-layers on Cu(111) surface

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Progress in the ability of understanding tribological properties in adsorbed film systems is of paramount importance to unravel fundamental issues in the emerging field of nanoscale science and technology. Many extensive studies have used a quartz-crystal microbalance (QCM) to measure the friction between adsorbed layers and crystalline substrates. In this work, we report a theoretical investigation of the tribological behavior for solid Xenon monolayers physisorbed on the Cu(111) surface; this sliding interface has been recently investigated experimentally by Coffey and Krim [1]. In order to get a reliable description of the adsorbate/substrate interaction, we evaluate the potential energy landscape experienced by a Xe atom physisorbed on the Cu(111) surface by ab initio calculations. The static frictional properties are analyzed in details as a function of system temperature, presence of interlayer defects, load and the connected change of anticorrugation. Contrary to the QCM experimental results, we find that, due to perfect interface commensurability, the (full monolayer) system exhibits strong pinning. However, the numerical simulations suggests that the simultaneous presence of thermal effects and of interlayer defects, lowering significantly the activation energy barrier, causes a considerable reduction of the static friction threshold. An unexpected dependence on load is also predicted and related to the characteristic anticorrugation features of the Xe/Cu interaction. The mechanisms of dissipation during sliding are investigated by measuring the slip time.

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Understanding the cleavage of diamond from the bond breaking

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First principles simulations provide the basis for the critical assessment of the different mechanisms proposed so far to explain the highly selective preference of diamond to fracture in the {111} set of planes. Our crack tip stability calculations for different crack orientations in the (111) and (110) planes show that cleavage in diamond is controlled by energy barriers to bond breaking that lead to lattice trapping of the crack. This conclusion is also supported by the differences found between the (111)and the other low-index diamond planes in the cohesive force function, calculated as the distance derivative of the energy per unit area required to separate two rigid slabs along their surface normals. This approach, that focuses on the accurate determination of the bond force non-linearity, provides an alternative to full fracture simulations in order to characterize the lattice trapping, and thus, the fracture behavior of materials.

Towards the synthesis of fullerenes: triazafullerene adsorption on noble metal close packed surfaces

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Combining STM, XPS and NEXAFS measurements with first principles calculations, we study the adsorption of C57H33N3 on Au(111) and Pt(111) surfaces, and the possibility of closed fullerene formation by thermal annealing using these molecules as precursors. For room temperature deposition and molecular coverages from 0.1 ML to 5 ML, we found that the molecules diffuse on the Au(111) surface and thermal annealing (uo to 800 K) leads to occasional formation of triazafullerenes C57H2N3. When Pt(111) is used as substrate, the molecule is well anchored to the surface at room temperature, rending possible the observation of molecular orbitals, and the formation efficiency is close to 90% at 675 K. Large scale first principles local orbital DFT calculations, provide insight into these experimental results. Differences in mobility on Au(111) and Pt(111) are explained by the adsorption energetics, and traced back to the different surface reactivity. Molecular dynamics simulations, based on temperature-induced deshydrogenation, suggest a possible pathway for the formation of closed fullerenes.

First-principles study of the cubic-SiC(100) - 4x2 surface

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We investigate the atomic scale structure and electronic properties of the Si-terminated SiC(001)-c(4x2) surface of cubic silicon carbide. This surface is known to undergo a reversible c(4x2) ↔ (2x1) phase transition at a temperature near 400 o C. The atomic structure of the low tempara-ture phase, i.e. the β-SiC(001)-c(4x2) surface, is still under strong debate. Two are the main models under discussion: in the first model, proposed on the basis of experimental STM images, Si atoms form Si-Si dimer rows having alternatively up and down dimers (AUDD) [1]. The second model, the missing row asymmetric dimer (MRAD) model, was suggested on the basis of first-principles total energy calculations [2]. We have analyzed using an efficient first-principles molecular dynamics technique [3] these atomic models, as well as possible variants, obtaining two other atomic structures that are competitive with the AUDD and MRAD models. In order to discriminate between these four atomic models we have also calculated their corresponding theoretical STM images, that are compared in detail with the experimental evidence [1].

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Density functional embedding for molecular systems

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We introduce a density functional based embedding method for the study of molecular systems in condensed phase. The system is partitioned in molecular subunits, which are individually treated by standard Kohn–Sham method by calculating the electronic density on small molecular grids. The necessary correction to include intermolecular interactions is introduced by an embedding potential derived from orbital-free density functional theory, by using kinetic energy functionals. The method leads to a linear scaling electronic structure approach that maps naturally onto massively parallel computers. Molecular dynamics simulations of water at room conditions result in a liquid with unstructured second solvation shell. The application to more weakly interacting molecular systems, like liquid acetronile, shows extremely satisfactory agreement between the full KS approach and the embedding approach. Improvements of the methodology should consider the neglected orthogonality condition betweem molecular orbitals belonging to differen molecular units. Extentions of the method will address the calculation of properties (spectroscopy) and the application to solid state.

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Enhanced chemical reactivity of gold nanowires

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Formation, exceptional stability and structure of pure one-dimensional gold atomic chains has been received a lot of attention last years. Experimental measurements show as significant changes of the conductance properties of atomic chains in presence of H_2 atmosphere [1] and recently work [2] reports experimental evidence for atomic chain formation strongly enhanced due to oxygen incorporation. For detail insight, we have carried out extensive first principles simulations, using fast local orbital DFT code FIREBALL, of the whole stretching process of Au nanocontacts combined with a Keldysh-Green's function approach for the electronic transport [3]. Our first principles simulations of the deformation path of a clean gold atomic contact show gradual formation of a mono-atomic chain with up to 4 atoms. As second step, we have studied possible adsorption and dissociation processes of H_2 molecule. In addition, we have performed simulations of the deformation process of Au nanocontact with oxygen molecule/atom to find possible tendency to be incorporated into the chain during the elongation process. In the case of H_2 molecule, our results [4] show how the molecule tends to dissociate on the Au chains and reduces significantly the conductance to values around ∼0.6 G0 in very good agreement to experimental values [2]. In the case of O_2 , we observe an incorporation of the molecule into the mono-atomic chain along the stretching process forming longer chains according to the experimental observations [2]. Both cases point out strong chemical reactivity of gold atomic chain, in contradiction to well known nobility of gold material [5].

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Interstitials in FeCr studied by Density Functional Theory

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Density Functional Theory calculations have been used to study relaxed interstitial configurations in FeCr alloys. The ionic and electronic ground state of 63 interstitial structures has been determined. Interstitials were placed in FeCr alloys with 9 to 14 atom percent Cr in which the Cr atoms were either monatomically dispersed or clustered together. The distance between the interstitials and Cr atoms was varied within the 4x4x4 bcc unit cell supercells. It is shown that Cr atoms at some distance from the interstitial can still influence the interstitial formation energy considerably. The multi-body nature of the Cr-Cr interactions in FeCr causes the Cr-interstitial interaction to be strongly concentration-dependent. Cr-interstitial binding energies calculated at dilute Cr concentrations can change by up to 0.5 eV and even change sign when recalculated at higher Cr concentrations. Determining the exact nature of the Cr-interstitial interaction is further complicated by the fact that FeCr alloying effects contribute more to the total formation energy than Cr-interstitial interactions. The long-range influence is not due to the interstitial strain field protruding into Cr-rich parts of the supercells. Instead, it is possible that some aspect of the electronic structure is responsible for changing the formation energies, although the Fermi-level and band energies were found not be the sole governing parameter. Our observations are likely to prove a serious challenge in the construction of FeCr force field potentials. Some patterns should not be too difficult for any potential to reproduce, e. g. the energy differences between different dumbbell orientations are quite independent from the configuration of Cr atoms that are slightly further away from the interstitial. Also, Cr atoms that are slightly further away from the interstitials seem to have little influcence on any aspect of the interstitial, as long as they are clustered together. However, monatomically dispersed Cr atoms do have a strong, long-range influence on the interstitials, so any empirical potential should not only be concentration-dependent, but should also be aware of the clustered/dispersed nature of the Cr. This observation, combined with the long-range, multibody, concentration-dependent nature of the Cr interactions will likely prove difficult to reproduce with a computationally cheap empirical potential.

Hydrogen damage in metals: Constrained molecular dynamics and Monte Carlo simulations of Superabundant vacancies

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Study of In adsorption on a In-rich a2(2x4) InGaAs surface on GaAs(001)

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The study of adatom diffusion and island nucleation on surfaces is a fundamental step to understand thin layer formation and morphology. In particular, it can shed light on the formation mechanisms of self-assembled nanostructures on surfaces. Here, we address one of the most studied systems: InAs quantum dots grown on a GaAs(100) substrate [2,3], where the lattice mismatch between InAs and GaAs is of the order of 7%. The calculation of the surface diffusion coefficient is a problem often tackled using multi-scale modeling approaches. The energy barriers between the adatom adsorption sites are calculated within a first-principles approach using a wide set of DFT calculations, while the diffusion simulation over larger time and space scales is then performed using a kinetic Monte Carlo Method. The first step is to calculate the surface equilibrium structure and the adatom adsorption sites as a function of the composition and related stress of the surface. We have considered a InAs layer, of thickness 1.75 monolayer (ML), grown on a GaAs(001) buffer. The surface is a2(2x4) reconstructed, that is supposed to be the stable reconstruction for a compressively strained InAs, such is the considered layer when the InAs deposition exceeds 1 ML [4]. The first-principles pseudopotential calculations were performed using the ESPRESSO simulation package. We have investigated the potential energy surface (PES) experienced by the In adatom, finding three adsorption sites and have calculated the potential barriers between them. The most stable adsorption site is found when the In adatom can bond to the As in-dimer on one side and to one surface In atom on the other side, thus saturating three bonds and completing the cation last layer. These results will be then used to simulate In surface diffusion.

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Effects of impurities on cohesion at $\Sigma 5(210)$ grain boundary of magnetic metals

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Impurities at grain boundaries can lead to embrittlement or to strengthening of the material. We have studied the B, N and O impurities placed in interstitial and substitutional positions at symmetric $\Sigma 5(210)$ Fe grain boundary (GB). The full relaxation of supercell shape and volume results in a stable asymmetric grain boundary. We found that nitrogen in both interstitial and substitutional position is a cohesion enhancers while oxygen and boron are embrittlers. In all cases we observe big shifts ($0.47\div 2.33$ \AA) of grains with respect to each other. The equilibrium distance between the grains is decreased for impurities in substitutional positions and increased for atoms in interstitial places with respect to the relaxed clean GB. The magnetic moments of Fe atoms at grain boundary are increased and they tend to the bulk value in the middle of the grain in an oscillatory way. We also present preliminary results on grain boundary cohesion in antiferromagnet chromium.

From individual defects to microstructures

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I will discuss the assemblage of a multiscale strategy for the study of microstructure evolution in polycrystalline materials. Starting from atomistic models of isolated defects (dislocations, grain boundaries, microcracks, etc.), a hierarchy is constructed to obtain the time and length scale parameters for collective degrees of freedoms. The latter describe the defects and their interaction, in a class of mesoscale models based on a variational formulation of the dissipated power.

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Computational tools for modeling and simulation of nanoscale systems

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We present various computational tools that can aid research of nanoscale systems, by providing concrete examples of multiscale modeling workflows, in which mesoscale models are contructed from atomistic data, and mesoscale simulation methods are used to generate input for finite-element calculations. The link between the micro- and mesoscale is discussed into more detail, in particular the coarse-graining route via the Flory-Huggins theory of mixtures. We investigate a simple method to estimate the Flory-Huggins interaction parameters from force field calculations, based on sampling the density-of-states of molecular clusters in the space spanned by coarse-grained coordinates. We show how we use the density-of-states to calculate the excess free energy of mixing, and how this leads to mesoscale interaction parameters.

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Metal adhesion at oxide ceramic interfaces

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Heterogenous metal-ceramic systems are employed in multifunctional devices, which exploit the properties of composite materials formed by dissimilar constituents. In these materials the interface strength is crucial in determining the macroscopic properties and therefore they are significantly dependent on interface adhesion. We have performed an ab-initio systematic investigation of the interface properties and adhesion between transition metals and oxide ceramics, which allows us to extract qualitative trends on the dependence of the adhesion on the structure, stability and metal electronic charge

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Relaxation of semiconductor interfaces by molecular dynamics using enhanced bond order potentials

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Accurate empirical potentials are needed to study atomic processes via molecular dynamics (MD) simulations at time and length scales relevant for nanoscopic processes such as surface interaction during wafer bonding or relaxation of quantum dots.

Starting from the tight binding model (TB) an analytical expression for the bond order potential (BOP) is derived, which is related to the electronic density. In the crystal the attraction due to formation of electronic bonds is balanced by the repulsion (overlap & coulomb) as well as the energetic penalty incurred by electronic promotion. The analytic derivative of this cohesive energy describes the forces acting on each atom, which are then used to integrate the Newtonian equations of motion to study the MD. Expression for the σ bond order has been improved by including intermediate π bonds and on-site cross terms. Along with the coordination-dependent expression proposed for the promotion energy, the BOP4^+ with 4^{th} moments of the density accurately describes covalent bonds while scaling linear with the system size.

MD simulations applying BOP4^+ to study the generation of wafer bonded interfaces, which is like a crack closure process influenced by the surface step structure, roughness, defects, adsorbates, and the misalignment of the wafers, demonstrate the validity and advantage of the new potential.

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Multiscale Hybrid Simulations of Brittle Fracture

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The Learn on the Fly (LOTF) molecular dynamics scheme, which combines quantum-mechanical embedding and classical force model optimisation is applied to the brittle fracture of silicon. Dynamical simulations of cracks moving in the (111) cleavage plane show a novel sub-critical crack tip reconstruction, similar to the Pandey 7-5 surface, that delays the onset of fracture by increasing the lattice trapping barrier.

This poses the question: what is the equilibrium shape of the crack-tip? There is a competition between the local chemical energy required to break bonds and the elastic energy recovered by the formation of such a reconstruction. Since the latter is distributed over thousands of atoms, hybrid simulation is the ideal tool to investigate such truly multiscale problems.

The LOTF method is also currently being applied to the fracture of diamond and of graphene sheets.

A cohesive zone model for stress corrosion cracking in ceramic polycrystals

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Fracture in oxyde based ceramics is time dependent and three regime can be distinguished: beyond a load threshold; (I) the crack velocity increases with the charge, (II) stabilizes and (III) unstable crack propagation takes place thus defining the material toughness. In the present study, we focus on the description of the regime I. While the bulk response is linear elastic at room temperature, the mechanism underlying rupture combines a chemical and a mechanical action at the crack tip. The time and temperature dependency originates from a reaction-rupture process which is both thermally activated and stress dependent. In the case of ceramics, the water is involved in the chemical effect for bond breaking through a molecular process proposed by Michalske (1983, JACS). We present a cohesive zone description for the time dependent reaction-rupture process. We then show some results related to the time dependent intergranular failure in a 2D polycrystal.

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2.2 ESF Psi-k Programme Workshop/Conference Announcements

2.2.1 Workshop on "Multiscale approach to alloys: advances and challenges"

First Announcement

June 17-19, Stockholm/Sigtuna, Sweden

http://www.sigtunahojden.se/

Organizers:

Igor A. Abrikosov, Linköpings University, Sweden
H. Dreysse, Universite Louis Pasteur, France;
G. Ceder, Massachusetts Institute of Tecnology, USA;
M. Asta, UC Davis, USA;
L. Dubrovinsky, Universität Bayreuth, German

Topic: The goal of the conference is to bring together leading experts working in the field of multiscale modeling for alloys, and to exchange the expertise on the recent advantages in the field, as well as to discuss challenges on the way to the development of a consistent set of tools for ab initio simulations of disordered materials at all levels, from the electronic structure towards the microstructure.

We also invite leading experimentalists in the fields of spectroscopy, nanoscience, structural chemistry, and geophysics, to establish closer links between theory and experiment.

Preliminary list of invited speakers:

G. M. Stocks (Oak Ridge National Laboratory, USA) - confirmed
C. Wolverton (Northwestern University, USA) - confirmed
A. Zunger (NREL, USA) - confirmed
B. Johansson (KTH, Sweden, and Sandvik Steel) - confirmed
H. Skriver (DTU, Denmark) - confirmed L. Vitos (Budapest, Hungary and Stockholm, Sweden) - confirmed
B. Gyorffy (University of Bristol, UK) - confirmed J. Neugebauer (Max-Planck-Institute, Dusseldorf, Germany) - confirmed
Derwyn Rowlands (University of Bristol, UK) - confirmed
Dario Alfe (University College London, UK)
H. Dreysse (Universite Louis Pasteur, France) - confirmed
M. Katsnelson (Nijmegen University, The Netherlands)
A. V. Ruban (KTH, Sweden) - confirmed
P. A. Korzhavyi (KTH, Sweden) - confirmed
S. I. Simak (Linköping University, Sweden)- confirmed
M. Asta (UC Davis, USA)
S. Lidin (Stockholm University, Sweden)

L. Dubrovinskii (Bayreuth, Germany) - confirmed
Axel van de Walle (Cal Tech, USA) - confirmed
M. Sluiter, (Delft, The Netherlands) - confirmed
H. Reichert (MPI Stuttgart, Germany) - confirmed
Bernd Schönfeld (ETH, Switzerland) - confirmed
Anton Van der Ven (University of Michigan, USA)
D. Johnson (UIUC, USA) - confirmed
D. Morgan (University of Wisconsin, USA)
Adam Kijena (Uniwersity of Wroclaw, Poland) - confirmed
M. Alatalo (Lappeenranta University of Technology, Finland) - confirmed
Nora de Leeuw (UCL, London, UK)
Dave Prior (Liverpool University, UK)
Tonci Balic-Zunic (University of Copenhagen, Denmark)
N. Dubrovinskaia (University of Heidelberg, Germany) - confirmed

In addition, we encourage participation of young researchers and PhD students.

For more information, and to submit your application for the participation in the conference please, visit

`http://cms.ifm.liu.se/theomod/theophys/intl._alloy_conference/`

or contact

Prof. Igor A. Abrikosov
Department of Physics, Chemistry and Biology (IFM)
Linköpings University, SE-581 83 Linköping, Sweden

e-mail: igor.abrikosov@ifm.liu.se

Deadline for abstract submission is April 16, 2007

2.2.2 Workshop on ”Advances in Continuum Quantum Monte Carlo Methods”

Location: CECAM, Lyon, France

Dates: Monday, August 27th - Friday, August 31st, 2007

Organizers: C. Filippi, M. Foulkes, and R. Needs

The focus of the workshop will be on current methodological developments in continuum quantum Monte Carlo methods, including efforts to incorporate molecular dynamics and improve geometry optimisation schemes, to find more efficient ways of optimising trial wave functions, and to develop new algorithms alternative to the fixed-node diffusion Monte Carlo method. Speakers involved in pushing the frontier of applications to complex systems will also be invited.

To apply, go to http://www.cecam.org/, select ”Workshops” in the ”Activities” section on the left-hand side of the page, and then click the ”Advances in Continuum Quantum Monte Carlo Methods” workshop announcement. This will take you to a description of the workshop and an online application form. Space at CECAM is limited and so we may not be able to accept everybody who applies.

If you would like to attend but cannot afford to do so, please let the organisers know. The financial support available is very limited, but it may be possible to help a few of the more junior attendees. There is no conference fee.

Junior US researchers should apply for NSF travel support via the web site

http://www.mcc.uiuc.edu/travel/

Claudia Filippi (filippi@lorentz.leidenuniv.nl)
Matthew Foulkes (wmc.foulkes@imperial.ac.uk)
Richard Needs (rn11@cam.ac.uk)

2.2.3 Workshop on "THEORY MEETS INDUSTRY"

WORKSHOP ANNOUNCEMENT

"THEORY MEETS INDUSTRY"
THE IMPACT OF DENSITY-FUNCTIONAL CALCULATIONS ON MATERIALS SCIENCE

JUNE 12-14, 2007
ERWIN-SCHRÖDINGER-INSTITUTE FOR MATHEMATICAL PHYSICS
Boltzmanngasse, A-1090 WIEN, AUSTRIA

sponsored by

Center for Computational Materials Science, Wien
Erwin Schrödinger Institute for Mathematical Physics, Wien
Wolfgang Pauli Institute, Wien
Universität Wien
ESF Research Programme "Towards Computational Materials Design"

Scientific Scope

In 1998 a workshop called "Theory Meets Industry" was held at the Technical University in Wien to celebrate the start of the Research Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behavior of Solids and Surfaces" sponsored by the European Research Foundation (ESF) - better known as the "psik-network". The aim of the workshop was to confront the potential of the ab-initio simulation codes developed in academia with the necessities arising from industrial research.

The Research Programme has been renewed under the title "Towards Atomistic Materials Design" and is now approaching the end of the second funding period. Everybody will agree that much progress has been realized since the 1998 workshop and that density-functional theory develops an increasingly important impact on materials research, not only in academia, but also in industry. Therefore it seems to be timely to organize a second workshop "Theory Meets Industry". The workshop will take place on June 12-14 in the Erwin-Schrödinger Institute in Wien. The scientific program will be planned by a Scientific Advisory Board (SAB) consisting of Risto Nieminen (TU Helsinki), Chris Wolverton (Ford Motors and NWU Evanston), Herve Toulhoat (Institut Francais du Petrole), Ryoji Asahi (Toyota), Erich Wimmer (Materials Design) and Jürgen Hafner (U Wien).

As for the previous meeting the aim will be to highlight the most recent progress in the development of ab-initio density-functional and post-DFT methods and in front-line applications in academia and to present recent achievements in industrial research. In addition speakers from industry are invited to articulate the needs in applied research which have not yet been met by the progress in theory. Attendance to the meeting will be restricted to about 60 persons, with the aim of an approximately equal representation of academia and industry.

Invited speakers include:
Georg Kresse (U Wien)
Chris Skylaris (U Southhampton)
Joost van de Vondele (U Zürich)
Karsten Held (MPI Stuttgart)
Emilio Artacho (U Cambridge)
Richard Needs (U Cambridge)
Xavier Gonze (U Louvain)
Peter Blaha (TU Wien)
Rajev Ahuja (U Uppsala)
Tomas Bucko (U Wien)
Laszlo Szunyogh (TU Budapest)
Chris van de Walle (U Santa Barbara)
Isao Tanaka (U Kyoto)
Jutta Rogal (FHI Berlin)
Gerd Ceder (MIT)
Lars Nordström (U Uppsala)
Martijn Marsman (U Wien)
Miguel Gosalvez (U Nagoya)
Ryoji Asahi (Toyota Research Laboratories)
Louis Hector (General Motors)
Kurt Stokbro (Atomistix)
Pascal Raybaud (Institut Francais du Petrole)
Sadasivan Shankar (Intel)
Clint Geller (Bechtel-Bettis)
Betty Coussens (DSM Research Laboratories)
Hansong Cheng (Air Products)
Petrie Steynberg (Sasol Technologies)
Berit Hinneman (Topsoe)
Christophe Domain (EDF)
Donald Siegel (Ford Motor Company)
Oleg Mryasov, Werner Scholz (Seagate)
Yasunari Zempo (Sumitomo Chemical)
Wolfgang Mannstadt (Schott)
Susanne Opalka (United Technologies Research)
Chris Wolverton (Northwestern U)

Additional contributions from both academia and industry are invited - because of the very tight program schedule, most contributed papers will be presented as posters. If you intend to participate at the workshop, please complete the registration form attached to this message and send it by email or fax to the workshop secretary, Mrs. Edith Wolfsgruber (email: edith.wolfsgruber@univie.ac.at, fax: +43-1-4277-9514). If you intend to submit a contribution, join an abstract (template appended) to your registration. The registration deadline is April 15. You will be notified of the acceptance of your registration/contribution before April 25.

Contact:
Prof. Jürgen Hafner
Fakultät für Physik and Center for Computational Materials Science
Universität Wien, Sensengasse 8/12, A-1090 WIEN, Austria
Tel.: +43-1-4277-51400 (direct), -51401 (secretary) FAX : +43-1-4277-9514
Email: juergen.hafner@univie.ac.at
www: http://cms.mpi.univie.ac.at/

REGISTRATION FORM
”THEORY MEETS INDUSTRY”
THE IMPACT OF DENSITY-FUNCTIONAL CALCULATIONS ON MATERIALS SCIENCE
JUNE 12-14, 2007
ERWIN-SCHRÖDINGER-INSTITUTE FOR MATHEMATICAL PHYSICS
Boltzmanngasse, A-1090 WIEN, AUSTRIA

Name :

Affiliation:

Address:

Email:

Accompanying person:

Hotel reservation required from June to June.
Single ○ Double ○ room.
We offer to make reservations in two very good hotels close to the conference location and to the Physics and Chemistry Departments of our University and only two tram stops from the city center. The rate is about 85 Euro/night for a single room, including breakfast. We offer to make a pre-reservation which you will have to guarantee with your credit card by contacting the hotel we will indicate.

I intend to present a poster contribution: ○ yes ○ no
Title of contribution:

An abstract of my contribution

○ is appended to this registration form

○ will be sent until April 15.

Abstracts can be submitted in pdf or doc format. The maximum lenght is 1 A4 page, with 12pt lettering. You will be notified of acceptance of your registration/contribution not later than April 25.

Please send your completed registration form to the workshop secretary, Mrs. Edith Wolfsgruber (email: edith.wolfsgruber@univie.ac.at, fax: +43-1-4277-9514) AS SOON AS POSSIBLE. June is touristic high season in Vienna and we have to fix the hotel reservations immediately.

2.2.4 Winter Workshop on Nanoscale Materials

'Towards reality in nanoscale materials'

December 10th - 12th, 2007

Levi, Finnish Lapland

We are organizing a workshop entitled 'Towards reality in nanoscale materials' on December 10th - 12th 2007. The workshop will be North of the arctic circle, in Levi, Finnish Lapland. Due to kind support from the Psi-k network, the Academy of Finland and the Finnish National Graduate School in Materials Science both participation and accommodation are free.

Online registration is now open, with a deadline of October 1st 2007.

The main topics of the conference are:

* Application of first principles methods to atomistic modeling of non-ideal nanoscale materials
* Multiscale approaches to link first principles calculations to larger scale methods, such as kinetic Monte Carlo
* Defects in nano-structured carbon materials
* Surface chemistry at the nanoscale
* Defect creation - studies of doped and irradiated nanoscale materials
* Atomic scale control: charging and optical excitation of nanoparticels; mechanical manipulation

For details see: `http://www.fyslab.hut.fi/~tjh/workshop07.html`

Adam Foster
Arkady Krasheninnikov
Risto Nieminen

2.2.5 Joint CECAM/Psi-k Workshop on "Maximally-Localized Wannier Functions: Concepts, Applications, and Beyond"

CECAM, Lyon, France

Wednesday June 27 - Friday June 29, 2007

We have the pleasure to announce a joint CECAM/Psi-k workshop on

"Maximally-Localized Wannier Functions: Concepts, Applications, and Beyond",

that will take place in CECAM, Lyon (France), from Wednesday June 27 to Friday June 29 2007.

Please refer to the CECAM webpage www.cecam.fr (under Workshops) for additional information.

Interested participants are welcome to register at the CECAM web page. Due to limited space availability, the committee will need to operate a selection; acceptance will be notified at the end of April.

A one-day tutorial on the use of the PWSCF and Wannier90 electronic-structure codes to calculate maximally-localized Wannier functions and related quantitities will be offered on June 26; interested participants are welcome to contact directly Nicola Marzari (marzari@mit.edu).

Nicola Marzari, Alfredo Pasquarello, Ivo Souza

3 EU-Funded Marie Curie Conferences and Training Courses

3.1 CECAM Tutorial on the Siesta Code

Efficient density-functional calculations with atomic orbitals: a hands-on tutorial on the SIESTA code”

CECAM, Lyon (France)

June 18-22, 2007

This is a five-day hands-on tutorial on the use of the Siesta code (www.uam.es/siesta), aimed at researchers from different disciplines who want to use the code in their research and need, apart from basic practice, a grounding on the capabilities of the method and the approximations used. The main goal is that the students understand the physical and main technical approximations behind the method and can assess its reliability and its usefulness for a particular problem. Apart from the basics of density-functional theory, molecular dynamics simulation and geometry relaxation, which are common to most codes, the specific Siesta topics to be covered are the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, localization issues for linear scaling both in the computation of the matrix elements and in the resolution of the hamiltonian, as well as more technical ones such as the influence of the real-space grid and parallelization. The tutorial will consist of morning lectures followed in the afternoon by practical ”hands-on” sessions. Some fundamental knowledge of quantum mechanics will be assumed, as well as basic statistical mechanics for the molecular dynamics part. Some solid state physics background will be helpful but not strictly needed. Basic knowledge of UNIX is required.

Application procedure:

To be properly considered, all applications have to be entered directly on CECAM’s website (www.cecam.fr), after a login to the restricted area (upper right-hand corner). You can use the following link to go directly to the tutorial page:

`http://www.cecam.fr/index.php?content=activities/tutorial&action=details&wid=141`

The tutorial is supported by a Marie Curie grant from the European Union. The EU mandates that all applicants be classified according to their research experience, nationality, and age, and these factors will affect the admission criteria and the level of support. It is then particularly important that all relevant fields in the CECAM application form are filled out carefully. In particular, note that the measure of research experience is based on the date of the degree (B.Sc., master, etc) that gives access to doctoral studies.

Economy-class travel and lodging costs will be covered by CECAM for eligible participants. Accomodation for the students will be handled directly by CECAM.

Organizers:

Javier Junquera, Univ. Cantabria, Spain (javier.junquera@unican.es); Alberto Garcia, Inst. Ciencia Materials de Barcelona (albertog@icmab.es)

4 News from UK's CCP9 Programme

UK's Collaborative Computational Project 9 (CCP9) on "Computational Studies of the Electronic Structure of Solids"

4.1 Reports on the CCP9 Workshops

4.1.1 Report on AIMPRO Code Meeting

University of Exeter, Exeter, U. K.

12-13 December, 2006

The meeting was organised by R Jones and held at the University of Exeter. Three of the main themes for the workshop were *screened exchange theory*, *transfer doping and electrochemistry*, and *carbon related materials*. In addition, the workshop gave users an opportunity to learn techniques to solve run-time problems.

Malcolm Heggie (Sussex) explained the importance of the buckling of graphite layers and its implication for radiation damage. This was followed by calculations of Gianluca Savini (Sussex) which indicated that these could could account for the discrepancy between theoretical and experimental elastic constants of graphite. The effect of high temperatures on the formation energy of defects in graphite were presented by Gemma Haffenden (Sussex).

Chris Ewels (Nantes) gave a review on hybrid methods to determine migration barriers and applied these to the problem of BN nanotubes. Bob Jones talked on and electrochemical issues at surfaces of diamond and InN. This was developed by Steve Sque's talk on electron transfer between nanotubes and diamond. Similar problems were outlined in a talk by Sven Oberg (Lulea) who compared traditional Hartree Fock packages with density functional ones for complex organic molecules on mineral surfaces. Richard Eyre (Newcastle) showed that alkyl groups behaved differently when adsorbed on nanocrystalline Si.

A number of other applications were described: Arnaud Marmier (Exeter) gave a talk on his recent finding that PtS exhibited negative compressibility. Jose Coutinho dealt with defects in Ge approached using clusters and Naomi Fujita gave an overview of modelling point and extended defects.

Patrick Briddon outlined new technique enabling forces due to shape changes to unit cells to be found ad well as describing advances in determining the magnetic properties of supercells and molecular clusters. Ben Hourahine gave a review of LDA+U theory and its incorporation into the DFTB code. Finally, Huda El Mubarek (Southampton) gave an experimentalists viewpoint of important problems relating to ion implantation damage in Si. The workshop achieved its aim to deal with new applications and new, as well as improved, functionality for density functional based codes.

Tuesday, 12.12.2006

Time	Speaker	Title
09:00-10:30	Patrick Briddon	Developments in Aimpro
10:30-11:00		*coffee break*
11:00-11:30	Thomas Eberlein	Screened exchange in AIMPRO
11:30-11:50	Alexandra Carvalho	Screened exchange method - a new approach to study defects in Ge
11:50-12:30	users	user discussion on AIMPRO
12:30-13:50		*lunch break*
13:50-14:00		meet outside the physics building for conference picture
14:00-14:20	Gemma Haffenden	LVMs and entropy of defects in carbon materials
14:20-14:40	Gianluca Savini	Mesoscale elastic constants in graphite
14:40-15:30	Ben Hourahine	News from the DFTB world
15:30-16:00		*coffee break*
16:00-16:20	Josep Campanera-A.	Density-functional calculations on the intricacies of the moir patterns
16:20-16:45	Jose Coutinho	Electronic structure of donor-vacancy aggregates in Ge
16:45-17:05	Huda El Mubarek	A new solution to the problem of dopant diffusion in semiconductor devices

Wednesday, 13.12.2006

Time	Speaker	Title
10:00-10:40	Bob Jones	Electrochemical reactions
10:40-11:00	Naomi Fujita	Point and extended defects in group IV materials
11:00-11:30		*coffee break*
11:30-12:05	Sven berg	AIMPRO compared with traditional quantum chemistry methods
12:05-12:20	Steve Sque	Using AIMPRO to model graphene and graphite
12:20-12:50	Malcolm Heggie	Ruck, tuck and buckle - a pile up of ideas for graphite
12:50-13:00	users	user discussion on graphite
13:00-14:00		*lunch break*
14:00-14:20	Luke Hounsome	The interaction of nitrogen with vacancy disks in diamond
14:20-14:40	Chris Ewels	Hybrid methods for determining migration barriers
14:40-15:00	Colin Janke	Properties of arsenic-vacancy related defects in silicon
15:00-15:30	Steve Sque	Modelling doped carbon nanotubes on hydrogen-terminated diamond
15:30-16:00		*coffee break*
16:00-16:30	Arnaud Marmier	Metamaterials and DFT: Negative compressibility of Platinum Sulfide
16:30-16:50	Richard Eyre	Stability of short alkyl groups on bulk and nanocrystalline Si surfaces
16:50-17:20	Imad Belabbas	What do threading dislocation cores look like in wurtzite GaN?

List of Participants

Almeida, Luis	University of Aveiro, Portugal
Belabbas, Imad	University of Caen, France
Bichoutskaia, Elena	University of Cambridge, UK
Briddon, Patrick	University of Newcastle upon Tyne, UK
Campanera-Alsina, Josep	University of Sussex, UK
Carvalho, Ines	University of Exeter, UK
Coutinho, José	University of Aveiro, Portugal
Davidson, Calvin	University of Sussex, UK
Eberlein, Thomas	University of Exeter, UK
El Mubarek, Huda	University of Southampton, UK
Ewels, Chris	Institute of Materials, Nantes, France
Eyre, Richard	University of Newcastle upon Tyne, UK
Fujita, Naomi	University of Exeter, UK
Haffenden, Gemma	University of Sussex, UK
Heggie, Malcolm	University of Sussex, UK
Hounsome, Luke	University of Exeter, UK
Hourahine, Ben	University of Strathclyde, UK
Janke, Colin	University of Exeter, UK
Jones, Bob	University of Exeter, UK
Latham, Chris	UK
MacLeod, Robert	University of Newcastle upon Tyne, UK
Marmier, Arnaud	University of Exeter, UK
Öberg, Sven	Luleå University of Technology, Sweden
Savini, Gianluca	University of Sussex, UK
Sque, Steve	University of Exeter, UK
Suarez, Irene	University of Sussex, UK
Underwood, Jack	University of Exeter, UK
Zobelli, Alberto	University of Paris XI, Orsay, France

5 General Workshop/Conference Announcements

5.1 Announcement of Computational Summer School on "Quantum Monte Carlo from Minerals and Materials to Molecules" in Illinois

University of Illinois, July 9-19, 2007

Dear Colleague,

We are planning to hold a summer school on "Quantum Monte Carlo from Minerals and Materials to Molecules", July 9-19, 2007 at the University of Illinois. The aim is to bring together advanced undergraduates, graduate students and post-docs, faculty, and research scientists from the fields of geophysics, physics, chemistry, as well as materials science to learn about QMC calculations and their applications. The school will have lectures in the morning and interactive laboratories in the afternoon.

Preliminary list of presenters:

Dario Alfe, University College London
Michele Casula, University of Illinois
David Ceperley, University of Illinois
Ronald Cohen, Carnegie Institution of Washington
Neil Drummond, Cavendish Laboratory, University of Cambridge
Claudia Filippi, Universiteit Leiden
Richard Hennig, Cornell University
Jeongnim Kim, University of Illinois
Pablo Lopez Rios, Cavendish Laboratory, University of Cambridge
Burkhard Militzer, Carnegie Institution of Washington
Lubos Mitas, North Carolina State University
Lars Stixrude, University of Michigan
Cyrus Umrigar, Cornell University
Renata Wentzcovitch, University of Minnesota
Shiwei Zhang, College of William and Mary

Preliminary list of topics to be covered:

First principles calculation in geophysics
Equations of state, elasticity and thermal properties of solids
Introduction to Monte Carlo Methods
Variational Monte Carlo
Diffusion Monte Carlo
QMC applications in geophysics
Pseudopotential generation
Wavefunction optimization methods
Wavefunction using pfaffians and backflow
Path integral Monte Carlo
Auxiliary field methods

Please consult the website

http://www.mcc.uiuc.edu/summerschool/2007/qmc

for up-to-date information on the instructors, topics and application materials.

We would like your opinions on the workshop topics to make sure that the needs of the prospective students and the QMC community will be met. Please take a few minutes to respond to our email.

How many people at your institution could attend during this time period, assuming that they are not limited by funding? (Note that there will be a $75 registration fee. Housing will be provided at no cost for off-campus participants, and particpants can apply for travel support.)

What topics would be essential or desirable to include for these participants?

Thank you,

Organizing Committee:

David Ceperley, Burkhard Militzer, Ronald Cohen, Richard Martin and Jeongnim Kim

This school is supported by NSF-EAR 05-30282, NSF-EAR 05-30643 and the Materials Computation Center NSF DMR-03-25939 ITR.

5.2 Windsor Summer School on Condensed Matter Theory - 2007

6-18 August, 2007

Windsor Great Park, Windsor, U. K.

Dear Colleagues,

Please, bring attention of PhD students and junior postdocs in your group to the 4th International Windsor Summer School on Condensed Matter Theory "Quantum Transport and Dynamics in Nanostructures" co-organised by V. Falko (Lancaster), V. Kravtsov (ICTP Trieste), I. Lerner (Birmingham), P. Littlewood (Cambridge) and J. von Delft (LMU Munchen).

This School will take place 6-18 August, 2007 in the Cumberland Lodge, Windsor Great Park, Windsor, and it will review the state of the art in theory and experiment on quantum nano-systems and nanostructured materials. Thanks to the EPSRC and IoP support, we shall be able to finance (at least, partially) the attendance of young researchers from the UK (at least, 50% of the cost of full-board accommodation).

The Windsor School courses will cover the following topics: Electronic properties of the recently discovered new 2D material - graphene; review of recent progress in quantum Hall effect and spin-Hall effect in novel semiconductor structures; The bosonisation technique and functional renormalisation group methods in application to the Kondo effect, Luttinger liquids in quantum wires and carbon nanotubes; Theory of quantum information processing, phase coherence and de-coherence in qubits, coherent exciton dynamics and optical properties of quantum dots in microcavities; Adiabatic and non-adiabatic dynamics of quantum condensates of finite dimensions.

Lectures in theoretical methods will be complemented by reviews of advanced experiments and focused research seminars. Lectures and seminars will be given by

B. Altshuler (Columbia U, NY),
I. Aleiner (Columbia U, NY),
C. Bennett (IBM),
A. Briggs (Oxford),
M. Buttiker (Geneve),
V. Cheianov (Lancaster),
M. Dresselhaus (MIT),
A. Geim (Manchester),
D. Haldane (Princeton),
B. Halperin (Harvard),
A. Imamoglu (ETH, Zurich),
M. Kastner (MIT),
C. Marcus (Harvard),
C. Marrrows (Leeds),
V. Meden (Gottingen),
W. Metzner (MPI-Stuttgart),

and by the organisers.

Deadline for applications will be 15 May, 2007.

Cost of full-board accommodation at Cumberland Lodge, in shared twin room: 70 GBP. Registration fee: 9 GBP if paid by 15.06.07 (110GBP upon arrival).

Programme and on-line forms can be viewed at

http://www.lancs.ac.uk/users/esqn/windsor07 .

Prof. V. Falko
Physics Department
Lancaster University
Lancaster, LA1 4YB, U. K.

Tel: 01524 593180
Fax: 01524 844037

5.3 Conference on Computational Physics (CCP2007)

Universite Libre de Bruxelles, Belgium

September 5-8, 2007

The next conference in this world series will be held in Europe, at the Solbosch campus of the Universite Libre de Bruxelles in Brussels.

Every Sientisct or PhD Student interested in the conference is welcome.

This conference will concern various subfields in Physics, ranging from electronic structure computations to simulations in astrophysics. It is aiming at being the reference place for computational developments in physics.

There will be a special emphasis this year on condensed matter physics,

Electronic structure
Quantum Monte Carlo
Materials modelling
Soft matter and biomaterials
Non-equilibrium matter
Micro fluids
Mesoscopic modelling, etc., but other areas including
Astrophysics
Particle physics
Plasma physics

will be covered in parallel sessions.

There will also be sessions on

Methodological advances and Large-code development.

The conference chairman is Professor Michel Mareschal.

Since March 1st, 2007, the website of the conference has been open. All useful information is to be found at

http://ccp2007.ulb.ac.be

Note the closing date of 1.June for contributed talks and posters.

Quentin Knaepen
Conference Public Relations
CCP 2007 - Conference on Computational Physics
Physique des Polymeres
ULB Campus Plaine - CP 223
Boulevard du Triomphe
1050 Bruxelles
Tel : +32 (0)2 650 57 32
Fax : +32 (0)2 650 56 75
Email : qknaepen@ulb.ac.be

5.4 Gordon Research Conference on TDDFT

Gordon Research Conference: Time-Dependent Density-Functional Theory

http://www.grc.uri.edu/programs/2007/timeden.htm

July 15-20, 2007

Colby College, Waterville, Maine

Chairs: Carsten A. Ullrich and Kieron Burke
Co-Chair: Angel Rubio

Time-dependent density-functional theory (TDDFT) provides an efficient, elegant, and formally exact way of describing the dynamics of interacting many-body quantum systems, circumventing the need for solving the full time-dependent Schrdinger equation. In the 20 years since it was first rigorously established in 1984, the field of TDDFT has made rapid and significant advances both formally as well as in terms of successful applications in chemistry, physics and materials science. Today, TDDFT has become the method of choice for calculating excitation energies of complex molecules, and is becoming increasingly popular for describing optical and spectroscopic properties of a variety of materials such as bulk solids, clusters and nanostructures. Other growing areas of applications of TDDFT are nonlinear dynamics of strongly excited electronic systems and molecular electronics.

The purpose and scope of this Gordon Research Conference is to provide a platform for discussing the current state of the art of the rapidly progressing, highly interdisciplinary field of TDDFT, to identify and debate open questions, and to point out new promising research directions.

The conference will bring together experts with a diverse background in chemistry, physics, and materials science.

Invited speakers and discussion leaders:

Roi Baer
Evert J. Baerends
Stefano Baroni
Andre Bandrauk
Harold Baranger
Thomas Brabec
Mark Casida
Roberto Car
James Chelikowsky
Giulia Galli
Fillipp Furche
Andreas Goerling
E.K.U. Gross
Stefan Kurth

David Langreth
Manfred Lein
Neepa Maitra
Miguel Marques
Nicola Marzari
Oleg Prezhdo
Lucia Reining
Angel Rubio
Tamar Seideman
Annabella Selloni
Tchavdar Todorov
Sergei Tretiak
Meta van Faassen
Troy Van Voorhis
Giovanni Vignale

We hope to see you at this meeting!

Registration deadline is June 24, but we encourage early registration since we expect the conference to be heavily oversubscribed.

Carsten A. Ullrich
Assistant Professor
Department of Physics & Astronomy
Office: 424 Physics University of Missouri
Columbia, MO 65211

Phone: (573) 882-2467, Fax: (573) 882-4195
e-mail: ullrichc@missouri.edu
`http://web.missouri.edu/~ullrichc`

5.5 Conference on ELECTRON MICROSCOPY AND MULTISCALE MODELLING

Moscow, Russia, September 3-7, 2007

http://www.crys.ras.ru/EMMM07/index.en.htm

EMAIL: emmm-07@ns.crys.ras.ru

Submission of abstracts until 10 May 2007

Reduced rate registration until 20 June 2007

This conference, sponsored by the International Union of Crystallography, will bring together experts in methods of interrogating structures at nano- and meso-scales, and multiscale materials modelling.

Topics of the conference include:

- electron diffraction imaging
- electron spectroscopy
- density functional methods
- structure of defects and dislocations
- dynamical properties of defects
- dislocation dynamics
- surfaces and defects on surfaces
- structure of grain boundaries
- atomistic modelling of diffusion of defects
- modelling microstructure on nano- and mesoscales
- imaging and spectroscopy of nanostructures
- magnetic effects in materials
- diffuse and small angle scattering
- charge density measurements
- advanced materials for power generation
- applications of electron microscopy
- neutron and X-ray diffraction methods

September is the best time for visiting the city of Moscow to enjoy the numerous sights and attractions that it has to offer.

We are looking forward to welcoming you to EMMM-07

Prof. Anatoly Avilov
emmm-07@ns.crys.ras.ru

Vice Chair, Organizing Committee of EMMM-2007, Institute of Crystallography, Russian Academy of Sciences, Leninsky Prospect, Moscow, Russian Federation

5.6 SNS2007 Conference

Second Circular

8th International Conference on Spectroscopies in Novel Superconductors (SNS2007)

August 20-24, 2007
Sendai, Japan

We are pleased to announce that the online application for the 8th International Conference on Spectroscopies in Novel Superconductors (SNS2007) is now available at the following website:

http://sns2007.imr.tohoku.ac.jp/

The deadline of the abstract submission is April 15, 2007.

Acceptance of your abstract will be informed around the end of April.

The registration and hotel reservation is available on the Conference website.

We would also appreciate it, if you could forward this message to colleagues who might be interested in SNS2007.

We look forward to meeting you at SNS2007 in Sendai.

Sadamichi Maekawa (Tohoku University)
Chair of SNS2007
E-mail: sns2007@imr.tohoku.ac.jp

5.7 14th WIEN2k hands on workshop on the WIEN2k package

Institute of High Performance Computing, Singapore

July 6-9, 2007

http://www.wien2k.at

The WIEN2k workshop will be held at the Institute of High Performance Computing (IHPC) Singapore, from 6th to 9th July 2007, as a post conference workshop to ICMAT 2007.

The WIEN2k programme package is one of the most popular DFT codes in Computational Materials Science and enables calculation of the electronic structure of solids with high precision. The WIEN2k workshop includes elementary and advanced tutorials on DFT, electronic structure calculations, magnetic, optical and transport properties as well as detailed introduction and hands-on exercises with the WIEN2k programme. In addition, there will also be oral and poster presentations given by selected participants.

Following a long tradition and with great vitality, the WIEN2k workshop provides an arena for new and experienced WIEN2k users to come together and discuss both elemental questions as well as the latest developments in the world of WIEN2k.

For more information go to http://www.wien2k.at

The tentative list of invited speakers includes:

-Prof. C. Ambrosch-Draxl (Univ. Leoben, Austria)
-Prof. P. Blaha (TU Vienna, Austria)
-Dr. R. Laskowski (TU Vienna, Austria)
-Dr. G. Madsen (Univ. Aarhus, Denmark)
-Prof. P. Novak (Prague)
-Prof. K. Schwarz (TU Vienna, Austria)

5.8 Symposium on "Electronic structure modeling of heterogeneous catalysis"

2007 Fall annual meeting of the American Chemical Society

August 19-23, 2007, Boston, U. S. A.

We would like to draw your attention to a symposium we are organizing on "Electronic structure modeling of heterogeneous catalysis", for the 2007 Fall Annual Meeting of the American Chemical Society.

The symposium will bring together researchers who are using a variety of techniques - based on first-principles electronic-structure approaches - to describe the thermodynamics and kinetics of heterogenous catalysis, in ultra-high vacuum or under realistic conditions. Talks appropriate to the symposium will cover areas as diverse as exchange-correlation functionals and metal-molecule interactions, simulations in the presence of solvents or an electrochemical potential, electron-transfer reactions, kinetic Monte Carlo or multiscale modeling of catalytic reactions, materials optimization and design for heterogeneous catalysis - to name a few.

The firm deadline for the submission of contributed abstracts was April 2, 2007; with abstracts submitted directly to

http://oasys.acs.org/acs/234nm/oasys.htm

Nicola Marzari
Department of Materials Science and Engineering Massachusetts Institute of Technology

Andrzej Wieckowski
Department of Chemistry
University of Illinois - Urbana champaign

6 General Job Announcements

Postdoctoral Position for theoretical research on magnetoelectrics

Institut de Ciencia de Materials de Barcelona, Spain

One post-doctoral position is available, with Jorge Íñiguez at the ICMAB-CSIC in Barcelona (http://www.icmab.es/dmmis/leem/jorge), to conduct theoretical research on magnetoelectric systems.

Research project

The research project concerns the quantum theory and modeling of magnetoelectric materials. It will take place in the context of the ongoing MaCoMuFi project (http://www.macomufi.eu) that involves the leading experimental groups in the field in Europe, as well as the theory groups in Barcelona and Liege (Philippe Ghosez, http://www.phythema.ulg.ac.be/Personnes/ghosez.htm). The work will involve frequent interaction with the theory group in Liege, as well as with the experimental groups of MaCoMuFi.

Practical aspects

The initial contract will be for one year starting at the earliest convenience of the candidate, with possible renewals up to 2 or 3 years.

Candidates

The candidates should have experience with first-principles computational methods. Previous work on strongly-correlated systems and development of first-principles methods will be highly valued.

Application

Candidates can send (i) a letter of motivation, (ii) a CV and (iii) two recommendation letters to Dr. Jorge Iñiguez (jiniguez@icmab.es).

Jorge Iñiguez - Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC, Spain), Laboratory of Electronic Structure of Materials

Post-Doctoral Position:
Institut Charles Gerhardt, Montpellier, France

Start: before December 2007

Duration: 12 months (funded by french ANR projects)

Two postdoctoral positions are immediately available in the Theoretical Chemistry group of the Institut Charles Gerhardt in Montpellier (south of France). The proposals deal with electronic structure computations of periodic solids in the field of energy storage and photovoltaic, using first-principles density functional theory (codes VASP, Abinit, WIEN2K, ADF Band). The candidates will participate to the characterization of chemical bonds and to the determination of the thermodynamic magnitudes involved into the chemical/physical properties of the investigated materials, as well as to the analysis of surface interactions.

Candidates should have a solid background in quantum chemistry (molecular or solid) and in Density Functional Theory. Computer skills (Linux/Fortran) will be appreciated.

Applicant should send his/her curriculum vitae (including a statement of research interests) as well as two recommendation letters to:

Dr Marie-Liesse DOUBLET
Institut Charles Gerhardt
UMR5253 CNRS UM2-ENSCM-UM1
Equipe CTMM,CC14,
Universit de Montpellier 2
Place Eugne Bataillon 34095
Montpellier Cedex 5

Email : doublet@univ-montp2.fr

POSTDOCTORAL OPENING

Theoretical Chemistry of Surfaces, Interfaces and Catalysis

Laboratory of Chemistry, C.N.R.S.,
Ecole Normale Supérieure de Lyon, France

"Theoretical Insight in Selective Hydrogenation of Unsaturated Aldehydes in a Realistic Catalytic Environment"

A postdoctoral position is open in the field of theoretical modeling of reactivity at catalytic surfaces at the Laboratory of Chemistry of Ecole Normale Supérieure de Lyon, starting from September 2007.

In the recent years, the modeling of reactivity of multifunctional molecules at catalytic surfaces has been essentially performed by neglecting the influence of the catalyst support and of the solvent [1, 2]. However, it is well-known that the environment plays a critical role on the catalyst activity and selectivity. A probative example is the selective hydrogenation of unsaturated aldehydes (crotonaldehyde and prenal for citral fine chemistry) on platinum particles deposited on oxide supports (ceria, zirconia). Indeed, understanding the origin of the activity and selectivity requires a more realistic description of the metal/support interface, on one hand, and of the solvent/metal interaction, on the other hand.

In the Laboratory of Chemistry, the theory group has gained expertise throughout the years for adsorption properties and reactivity of organic molecules at metallic and oxide surfaces. In particular, the mechanism of a chemoregioselective reaction occuring at a metal surface has been recently elucidated by examining all the elementary steps at the atomistic level and by modeling kinetics [1, 2]. It is worth mentioning that our theoretical group is involved in several european research networks such as IDECAT, MONET, EUROSYM.

Hence, the successful post-doctoral candidate will tackle these complex systems on the basis of density-functional theory calculations (VASP program). The applicant should have a PhD in theoretical chemistry and/or condensed matter theory from a reputable higher education institution. Experience with DFT electronic structure calculations of periodic systems would be very helpful.

The project is part of a National Research Agency contract (SIRE, "SImulation of chemical REactivity at interfaces", other annoucements can be found at

http://perso.ens-lyon.fr/paul.fleurat-lessard/ANR)

in collaboration with three other French institutions (ENPC, IFP in Paris and LSDSMS in Montpellier). So the candidate is also expected to interact with these theoretical groups. The position is funded with a net salary of 2039 Euros per month.

The Ecole Normale Supérieure de Lyon provides an outstanding environment for research and teaching with a permanent staff of experts in chemistry and physics, and a continuously renewed staff of young graduate and postdoc researchers who wish to launch a successful career in these fields (see http://www.ens-lyon.fr for more details). Living in Lyon is also very nice and pleasant. The city is famous for its gastronomy.

Please send a cover letter and professional CV to Dr Françoise Delbecq or Dr David Loffreda at francoise.delbecq@ens-lyon.fr or David.Loffreda@ens-lyon.fr. Recommendation letters will be requested after a preliminary selection.

Dr David Loffreda
Laboratoire de Chimie, UMR CNRS 5182

Ecole Normale Supérieure de Lyon,
46 Allée d'Italie, F-69364 Lyon Cedex 07, France
tel: (+33) 4 72 72 88 43
fax: (+33) 4 72 72 88 60
email:David.Loffreda@ens-lyon.fr
http://perso.ens-lyon.fr/david.loffreda

Dr Françoise Delbecq
Laboratoire de Chimie, UMR CNRS 5182
Ecole Normale Supérieure de Lyon,
46 Allée d'Italie, F-69364 Lyon Cedex 07, France
tel: (+33) 4 72 72 88 43
fax: (+33) 4 72 72 88 60
email:francoise.delbecq@ens-lyon.fr

References

[1] Loffreda, D.; Delbecq, F.; Vigné, F.; Sautet, P. *Angwandte Chemie International Edition* **2005,** *44,* 5279.

[2] Loffreda, D.; Delbecq, F.; Vigné, F.; Sautet, P. *Journal of the American Chemical Society* **2006,** *128,* 1316.

Postdoctoral Position

Quantum chemistry. Dynamic Simulations.

Ab initio simulations of electrochemical processes in fuel cells

École Nationale des Ponts et Chaussées, PARIS, France

Electrochemistry is at the basis of a wide variety of chemical processes, including in particular energy generation in fuel cells. Due to the expected high impact of breakthroughs in fuel cell technology, many attempts to improve electrochemical processes in fuel cells are in progress. A number of them make use of ab initio simulations as a complement to, or a guideline for, experiments.

Yet, ab initio simulations in electrochemistry raise the issue of computing the electronic structure of a solid/solvent interface subjected to an electrostatic potential. The simulation methods available to date allow to impose the charge, hence only indirectly the potential. This way to proceed is not really applicable for the simulation of electrochemical reactions, for the latter usually take place at constant potential. Indeed, if one imposes the charge, the potential varies during the reaction process.

The purpose of this research project is to design, implement and test on benchmark examples, grand canonical self-consistent field (SCF) algorithms, in which the potential is held fixed, while the charge may change in the course of the iterations. This research project lays at the interface between applied mathematics and chemical physics and is jointly supervised by Eric Cancès (applied mathematics) and Jean-Sbastien Filhol (chemical physics). The host laboratory is the CERMICS (laboratory of applied mathematics, École Nationale des Ponts et Chaussées, located 25 minutes from the center of Paris, and easily accessible with public transportation). Monthly short stays at the ICG (Theoretical physics/chemistry group, Institut Charles Gerhardt, University of Montpellier, south of France) are scheduled.

Candidates must have a PhD in applied mathematics, physics or quantum chemistry, and an experience in computer programming (Fortran, C or C++).

This post-doctoral position is granted by the French research council ANR and is open from June 2007. The net salary is approximatively 2000 euros per month. The initial contract will be for one year, with possible renewal for a second year.

Applications (CV, letter of motivation and two recommendation letters) can be sent by e-mail to Prof. Eric Cancès (cances at cermics.enpc.fr)

This theoretical work is part of a new project funded by the French National Research Agency (ANR) within the framework of the High Performance Computing and Simulation Program. The other partners are laboratories with first class expertise in electronic structure calculation and applied mathematics. More details about the project and other available positions can be found at:

`http://perso.ens-lyon.fr/paul.fleurat-lessard/ANR`

Postdoctoral Position

Quantum chemistry. Dynamic Simulations.

Efficient methods to find reaction paths.

Chemistry Laboratory, École Normale Supérieure de Lyon, LYON,France

A post-doctoral position is available in the Chemistry department of the École Normale Supérieure (Lyon, France). The position is now open, and funded for 12 months from starting date. The net salary is approximately 2000 euros per month.

The successful candidate will develop and test methods to find reaction mechanisms at the microscopic level. These reaction paths should be determined both at 0K and at finite temperature, on the free energy surface. This project thus belongs to the more general topic of overcoming high barrier in the study of rare events. Development of news methods/algorithms lays at the interface between applied mathematics and chemical physics and will be jointly supervised by Paul Fleurat-Lessard (Chemical Physics) and Tony Lelièvre (applied mathematics). The host laboratory is the Chemistry Laboratory (Lyon). Short stays at the CERMICS (laboratory of applied mathematics, École Nationale des Ponts et Chaussées, Paris) are scheduled. These methods will be coupled to standard quantum chemistry packages as well as molecular dynamic codes. Besides simple test reactions, applications will include realistic models of complex systems used in aqueous electrochemistry and heterogeneous catalysis.

Applicants should hold a PhD in theoretical chemistry/physics, applied mathematics, or other related areas with a competitive track record. Candidates are required to have experience in numerical scientific computing, with quantum chemistry program packages or molecular dynamics packages. Experience of free energy calculations is desirable. Fluency in a high-level programming language, such as FORTRAN90 (preferred) or/and C/C++ is a requirement. Experience with parallel computing libraries, such as MPI, and extensive experience in a unix/linux environment is a definite advantage.

Motivated candidates are invited to send their CV, including a short motivation for carrying out this project, list of publications, abstract of research results (1 page) and two recommendation letters by e-mail (preferred format pdf or plain text) to

Paul.Fleurat-Lessard at ens-Lyon.fr

This theoretical work is part of a new project funded by the French National Research Agency (ANR) within the framework of the High Performance Computing and Simulation Program. The other partners are laboratories with first class expertise in electronic structure calculation and applied mathematics. More details about the project and other available positions can be found at:

`http://perso.ens-lyon.fr/paul.fleurat-lessard/ANR`

Post-doctoral Position in the Field of Ab Initio Spintronics

Institute of Physics and Chemistry of Materials of Strasbourg (IPCMS), France

A postdoctoral position is available immediately at the institute of physics and chemistry of materials of Strasbourg (IPCMS) in the field of ab initio electronic transport in organic/ferromagnetic tunnel junctions. The position is funded by a grant of the French research council ANR and can be renewed for up to three years. The IPCMS is a joint research center affiliated with the Centre National de Recherche Scientifique (CNRS) and with the University of Strasbourg. It currently employs 77 faculties and research staff. Experience in the field of ab initio electronic structure, electronic transport, and FORTRAN programming will be most useful. The successful candidate will work in the group of Mebarek Alouani (Professor), Olivier Bengone (Assistant Professor), Sebastien Lebegue (CNRS research staff), Carlo Massobrio (CNRS research staff), and Hugues Dreysse (Professor) and is expected also to collaborate with our strong experimental group in the field of spintronics at the nanoscale.

The application to this position together with a resume of recent research, a list of publications, and the names and emails of at least two referees should be sent by email to Prof. Mebarek Alouani (email: mea@ipcms.u-strasbg.fr).

Postdoctoral Position

Datamining and Computational Search for Self-healing Materials

Department of Materials Science, Delft University of Technology
Delft, The Netherlands

Applications are invited for a two-year post-doctoral position that is expected to become available as early as March 2007 but a later starting date is possible. The ideal candidate has experience in computational materials science. A PhD in materials science, physics, theoretical chemistry, or related field is required. The postdoc will perform a computational search for materials that can be used as transformation toughening dispersions in brittle materials. The search will utilize concepts from datamining and Pettifor structure maps. Moreover, contruction of a database using electronic density functional calculations is an essential part of this project. You will be interacting with a group of PhD students, postdocs, and staff so that good verbal communication skills in English are essential. The department of Materials Science at Delft University of Technology offers an exciting research environment with excellent facilities and working conditions.

Candidates should send a detailed resume including an outline of their research achievements and interests as well as contact information for academic references to

Marcel Sluiter
Virtual Materials Lab
Department of Materials Science
Delft University of Technology
Mekelweg 2, 2628 CD Delft
The Netherlands
Email:M.H.F.Sluiter@tudelft.nl

Consideration of candidates will begin immediately and continue until the position is filled.

Professorship in Theoretical Physics

The School of Engineering and Science at Jacobs University Bremen, Germany (formerly International University Bremen)

We invites applications for a professorship in theoretical physics beginning late August 2007. We are looking for applicants with strong research tracks in advanced Density Functional Methods with possible applications to nano-materials, hybrid interfaces and surfaces. Synergies with existing graduate programs, in particular with the Nanomolecular Science program, are expected. Candidates are expected to contribute to the undergraduate as well as graduate teaching. The teaching load is three courses per year. Strong research activities as well as close interaction with students inside and outside of class are expected. The language of instruction is English. Our students come from over 85 nations worldwide. Admission is highly selective. Salaries are internationally competitive. Initial contracts are for a period of seven years.

Applications including a curriculum vitae, list of publications, statements of research and teaching, and the names and addresses of at least three potential referees should be submitted no later than April 15th, 2007 to

Prof. Dr. Bernhard Kramer,
Dean of Engineering and Science,
Attn. Mrs Angela Schreiber,
Jacobs University Bremen,
P.O. Box 75 05 61,
28725 Bremen, Germany

Inquiries may be made by email to schreiber@iu-bremen.de.

For more information, see our website at

http://www.iu-bremen.de/schools/ses/physics/.

Online version of this job opening at

http://www.iu-bremen.de/about/jobs/11462/

Ph. D. Position

”Raman spectroscopy and ab initio calculations”

Laboratory of Condensed Matter Physics of the University of Metz (France)

We search for a suitable candidate for a Ph. D. position at the Laboratory of Condensed Matter Physics of the University of Metz (France) to whoever could be interested in this information. The candidate is expected to perform a combined experimental-theory work (Raman spectroscopy and first-principles calculations on lattice dynamics and ordering in mixed semiconductors) within the research context pursued in the laboratory - see the presentation of laboratory at

http://www.univ-metz.fr/recherche/presentation/pg-0013.pdf

The opening of the position depends on the availability of a suitable candidate, but is basically scheduled for September 2007. A suitable candidate could be of any nationality, but having obtained the degree equivalent of 2 years master (M2R, French Bac+5) in any country of the European Union, Albania, Andorra, Armenia, Azerbaijan, Bosnia and Herzegovina, Croatia, Georgia, Iceland, Lichtenstein, Macedonia, Moldova, Montenegro, Norway, Russian Federation, Serbia, Switzerland, Turkey, Ukraine, Vatican.

The command of French is advisable but not required.

The interested candidates are asked to contact

Prof. Olivier Pages (pages@univ-metz.fr)

and/or

Dr. Andrei Postnikov (postnikov@univ-metz.fr)
Tel. +33-387315873
Paul Verlaine University
Institute de Physique Electronique et Chimie
Laboratoire de Physique des Milieux Denses
1 Bd Arago
F-57078 Metz, France

PhD Studentships in Theoretical Nanoelectronics

Lancaster University, U. K.
Open to all EU students

Two fully-funded three year Ph. D. studentships are available in the Condensed Matter Theory Group at Lancaster University, under the supervision of Prof. Colin Lambert. The start date is any time between July 1st and October 1st 2007.

The successful applicants will join a multi-national research team working on quantum electron transport through nanoscale systems. Current projects include:

Single-molecules electronics, including single-molecule transistors and single-molecule sensors;

Giant magnetoresistance in spintronic devices, including semiconductor spin transistors and single-molecule spin valves;

Carbon based electronics, including carbon nanotubes, carbon ribbons and graphene

Electron transport through superconductng nanostructures including Andreev interferometers.

The appointees will have an opportunity to participate in a 4-institution EPSRC Basic Technology consortium ”Controlled Electron Transport Through Single Molecules” and a 12-institution EC network, ”Fundamentals of Nanoelectronics.”

Candidates should have, or be about to receive, a first class honours degree in theoretical physics. The studentships offer full costs (fees plus living expenses) for EU citizens for 3 years.

Further details may be obtained by contacting Prof Colin Lambert (C.Lambert@Lancaster.ac.uk)

or visiting the condensed matter theory web site:

http://www.lancs.ac.uk/depts/physics/research/condmatt/theory/tcmgroup.htm

Staff Research Position
Theoretical Condensed Matter Physics/Materials Science

Materials Theory Group

Materials Science and Technology Division
Oak Ridge National Laboratory, U.S.A.

Summary:

Applications are invited for a research staff member position in the Materials Theory Group at Oak Ridge National Laboratory. The successful applicant will be expected to significantly contribute to the science of materials theory and modeling within the Materials Theory Group (MTG) within the Materials Science and Technology (MST) Division. The MST Division encompasses one of the largest materials research efforts in the world. The Materials Theory Group has a staff of internationally recognized theoretical and computational physicists of which Dr. G. Malcolm Stocks is the current group leader. The successful applicant will be expected to contribute to the development of innovative theory and modeling programs and can expect the freedom to lead his/her own programmatic effort. He/she will have ample opportunity to interact with MST experimental groups engaged in the synthesis, characterization and development of a broad range of structural and functional materials. Additionally, unique opportunities exist for interaction with other theorists and experimentalists in the Center for Nanophase Materials Science, the Spallation Neutron Source (SNS), and the National Center for Computational Sciences. Interests in the development and application of ab initio electronic structure approaches for structural and/or functional materials and first principles electronic structure approaches for strongly correlated electron systems will be viewed favorably.

Responsibilities & Qualifications:

The successful candidate will have responsibility for contributing to the development of innovative theory and modeling programs within the MTG and to lead his/her own programmatic effort. A PhD in Theoretical Condensed Matter Physics/Materials Science is required and to qualify for this position you will have a strong publication record in theoretical condensed mater/materials science research. An appointment at a more senior level is possible for an exceptionally well qualified candidate. A strong interest and track record in the development and application of first principles electronic structure approaches to structural and/or functional materials properties is preferred. We also prefer experience in electronic structure approaches for strongly correlated electron systems, particularly as they relate to energy applications.

How to apply:

To apply for the position, please go to jobs.ornl.gov, select position #2239, Theoretical Condensed Matter Physics, Staff Research Position and submit your CV. For questions, please email an3@ornl.gov. Please submit your resume, references, and publication list in one file. We only accept Microsoft Word documents. If you have trouble applying for a position, please email Helpdesk@icims.com.

ORNL is a multi-program research facility managed by UT-Battelle for the Department of Energy. ORNL is an equal opportunity employer and committed to building and sustaining a culturally diverse workplace.

Postdoctoral Position
CEA, Bruyeres le Chatel, South of Paris, France

A postdoctoral position is available in the electronic structure group in the CEA (Bruyeres le Chatel, South of Paris, France) to work on the implementation and applications of both the LDA+U method and the combination of Density Functional Theory with Dynamical Mean Field Theory (LDA+DMFT). Applications on f-electrons systems are considered. This project will be carried out with several collaborators in the group. Supercomputer time will be available thanks to the supercomputers of the CEA.

Interested and motivated candidate should have obtained his PhD for less than two years and should have a solid background in solid state physics. He/she should have a good knowledge of Density Functional Theory, and/or Many Body Physics.

The contract is for one year, renewable upon mutual agreement. Applications are being considered now. The starting date will be between June 2007 and January 2008. Net Salary will be around 2100 euros a month.

Applicants should send a detailed CV, a letter of motivation, and the names of two references to Bernard Amadon (bernard.amadon@cea.fr) and Franois Jollet (francois.jollet@cea.fr)

For further informations, please contact:

Bernard Amadon
CEA/DIF
BP 12 - 91680 Bruyeres-le-Chatel
bernard.amadon@cea.fr

Three Postdoctoral Positions
SISSA International School for Advanced Studies, Trieste, Italy

Three postdoctoral positions are available immediately in the SISSA Condensed Matter Theory Sector in the following areas:

1) - "Ab initio calculations and strong correlations in magnetic nanocontacts" (E. Tosatti, A. Dal Corso, G.E. Santoro, M. Fabrizio)

2) - "Simulation and metadynamics applied to the structure of crystalline and amorphous clusters" (E. Tosatti, A. Laio)

3) - "Quantum Phase transitions and quantum annealing of disordered systems" (G.E. Santoro, R. Fazio)

Successful candidates will join a well established theoretical research group (http://www.sissa.it/cm/), with strong links to researchers at the Democritos National Center (www.democritos.it) and at the nearby International Centre for Theoretical Physics (www.ictp.it)

Candidates must hold a PhD in Physics or related discipline, and have good knowledge of, and some proven research experience with, pertinent theoretical and computational methods. electronic structure theory. Appointment is for two years and beginning of activity should be as early as possible.

Interested applicants should submit formal (paper) applications, complete with CV, publication list and a short (purely indicative) research program indicating which position is requested, as described in

`http://www.sissa.it/main/?p=A3_B4&id=220`,

arriving in SISSA not later than April 15, 2007. They should also arrange for no less than 2 reference letters to arrive within the same date.

Email contacts are welcome to principal investigators (scientific questions): tosatti@sissa.it, santoro@sissa.it, and to the Condensed Matter Secretary (administrative questions): bencina@sissa.it.

Postdoctoral Position

in Computational Condensed Matter Physics and Materials Science

DEMOCRITOS ”Modeling Center for Research in Atomistic Simulations”, Trieste, Italy

Applications are invited for one postdoctoral position available immediately within DEMOCRITOS ”Modeling Center for Research in Atomistic Simulations” in Trieste, Italy, extending on 1+1 years. The selected candidate will participate in a project aimed at developing and implementing new algorithms for the first-principles calculation of optical properties of nanostructured materials. This project is part of an ongoing collaboration between DEMOCRITOS and the Elettra Synchrotron Radiation Laboratory in Trieste and significant interaction with Elettra experimental groups is expected.

The candidate should hold a Ph.D. in the field either of theoretical physics/chemistry or materials science and have previous experience with first-principles methods as well as scientific programming.

Prospective applicants are requested to get in touch with Dr. Paolo Umari (umari@democritos.it, Democritos c/o Sincrotrone Trieste, Strada Statale 14 - km 163, 534012 Basovizza, Trieste ITALY) to whom they should submit a CV, including a list of publications, and at least the names of two referees (all this by e-mail).

Three Director Positions

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

The Ruhr University Bochum, Germany

The Ruhr University Bochum invites applications for the positions of

Three Directors (W3) of the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

in combination with Professorships in the areas of

Micromechanical modelling of macroscopic material behaviour: The main focus of this department is modelling material behaviour at the macroscopic scale. Continuum methods are extended and combined with atomistic and mesoscale concepts. A proven track record in research on mesoscale processes such as dislocation dynamics, texture evolution, microstructural damage accumulation and fracture mechanics is expected.

Scale-bridging thermodynamic and kinetic simulations at the mesoscopic scale: This department covers the mesoscale with special emphasis placed on microstructure, phase transformations, precipitation processes and interface dominated material properties. Simulation tools include statistical mechanics, Monte Carlo simulations and phase field modelling.

Simulation of material behaviour at the atomistic scale: The research objective of this department is the description of fundamental material properties, thermodynamic quantities and surface reactions at the atomistic scale. A strong focus on coupling atomistic level simulations to mesoscale materials properties is expected. Phenomena such as defect properties and microstructural evolution are in the focus of interest. Knowledge in the areas of DFT, empirical potentials and MD and/or the development of empirical potentials is required.

For all three positions (starting date: January 2008) proven track records in bridging length and time scales and the willingness to collaborate with the other two groups and with industry are expected. ICAMS is a newly founded interdisciplinary institute for modelling and simulation of advanced engineering materials including soft matter. ICAMS aims at predicting the macroscopic behaviour of engineering materials from atomistic properties and microstructure with the intention to provide tools allowing improved and accelerated development of new materials. ICAMS is funded and financed by leading German companies, the Federal State of North-Rhine Westfalia and the Ruhr University Bochum. ICAMS is designed to be a strong multidisciplinary centre consisting of three endowed chairs (encompassing several positions for research assistants and PhD students) and three associated advanced study groups which link ICAMS-activities with existing theoretical and experimental expertise. ICAMS' mission is to establish new research and educational programmes in the area of materials simulation, combining expertise from natural sciences, mathematics and engineering. ICAMS will have strong interactions with the material scientists at the Ruhr University Bochum, with leading institutes in materials research and with industry. ICAMS will also educate a new generation of materials engineers trained in advanced materials simulation techniques. We seek candidates with an outstanding international reputation, the ability to lead an institute and to collaborate with industry, experience in the acquisition of research funds and in teaching at the university level. The Ruhr University Bochum is committed to equal opportunity in employment and gender equality in its working environment. To increase equal gender distribution in all job categories and at all levels, we strongly encourage applications from qualified women. Female applicants will be given preferential consideration when their level of qualification, competence and professional achievements equals that of male candidates, unless arguments based on the personal background of a male co-applicant prevail. Applications from appropriately qualified handicapped persons are also encouraged.

Applications, including a curriculum vitae, a list of publications and a statement of research interests and plans, should be sent by April 13th, 2007 to: Dr. E. Weiler, Rector of the Ruhr University Bochum, concerning ICAMS, Ruhr-Universität Bochum, D-44780 Bochum. Potential candidates will be invited to participate in a scientific colloquium on 15th-17th of May 2007.

POST-DOCTORAL POSITIONS

COMPUTATIONAL MATERIALS THEORY

CALIFORNIA STATE UNIVERSITY NORTHRIDGE

Two postdoctoral positions are available in the W. M. Keck Computational Materials Theory Center at California State University Northridge (`http://www.csun.edu/~nkioussi/`) for research in

1) electronic structure and atomistic simulations of electromigration in nanowires and in

2) electronic transport of magnetic and multiferroic tunnel junctions and molecular spintronics.

Experience with first-principles electronic-structure calculations, electronic transport theory, and computer programming is required. It is expected that the candidate will develop further state-of-the-art first principles packages and apply them to problems of electromigration and spintronics. The research is in collaboration with both the Princeton Center for Complex Materials (Prof. R. Car) and UCLA (Profs. Ghoniem and King- Ning Tu).

Both positions are available immediately. Initial appointment is for one year, renewable for a second and/or third year (based upon satisfactory performance). Interested applicants should submit a curriculum vita, list of publications, and arrange to have two letters of reference sent to: Prof. Nicholas Kioussis, Department of Physics, California State University Northridge, 18111 Nordhoff Street, Northridge, CA 91330-8268 or via e-mail to: nick.kioussis@csun.edu. CSUN is an Affirmative Action, Equal Opportunity Employer.

Postdoc Position

Theoretical/computational solid state physics
University of Aarhus, Denmark

A 12 month postdoc position in theoretical condensed matter physics is vacant at the Department of Physics, University of Aarhus, Denmark. An applicant who is interested in joining current activities in calculations of optical properties including electron-hole correlations (solving the Bethe-Salpeter equation) will be preferred. Exprience with state-of-the-art electronic structure calculations is required.

Further information:

http://www.phys.au.dk/condensm

and by e-mail to nec@phys.au.dk.

Niels E. Christensen
Professor (Theor. Solid St. Physics)
Institute of Physics and Astronomy
Aarhus University
DK-8000 Aarhus C
Denmark
Tel.: (+45) 8942 3666
Fax : (+45) 8612 0740

POST-DOCTORAL POSITION

"Ab initio study of the effect of stresses on the stability of nano-precipitates in bcc-iron"
CIRIMAT/CNRS, Toulouse, France

An initially one-year postdoctoral position in physical metallurgy and condensed matter physics is available immediately at the CIRIMAT/CNRS, Toulouse, France.

Our team is participating in a three-year project on the effect of stresses on the nucleation kinetics of precipitates in steel and aluminum alloys. This project involves five French laboratories working in collaboration on the theoretical and experimental aspects of the subject.

The goal of the post-doctoral work in CIRIMAT will be to explain and model via ab initio calculations the stability of niobium nitride nanoprecipitates in a ferritic matrix. The challenge of this project is to take into account in a self-consistent way the role of the stresses induced by the presence of the precipitates in the matrix.

We are looking for a candidate having substantial experience in Density Functional Theory calculations, and a strong interest in materials science.

Interested candidates should submit their CV, including references and the list of publications to Dr. Philippe Maugis, CIRIMAT-ENSIACET, Toulouse, France, philippe.maugis@ensiacet.fr.

Postdoctoral Position

”Core structure and mobility of dislocations in hcp metals”

CEMES-CNRS, Toulouse, France

A two-year post-doctoral position is available starting on Sept. 1, 2007 at CEMES-CNRS, Toulouse (France).

The successful candidate will carry out numerical simulations of dislocations in hexagonal close packed metals such as titanium and zirconium. Besides a profound knowledge of condensed-matter theory, experience with first-principles electronic structure calculations or classical atomic scale simulations is required. The candidate will study the core structure of screw dislocations in hcp metals in different configurations and boundary conditions using first-principles DFT calculations. These results will then be used to test existing semi-empirical potentials and/or to construct new ones in order to study the dislocation mobility as a function of applied stress and temperature. This work is motivated by interesting and intriguing experimental results obtained on the dislocation mobility in Ti and Ti-Al at CEMES, Toulouse, by transmission electronic microscopy.

The candidate will work in the ”Crystallin Materials under Constraints” group of CEMES-CNRS, Toulouse (http://www.cemes.fr)and will be highly implicated in an ongoing collaboration with F. Willaime at SRMP, CEA/Saclay, France in the framework of the ANR (Agence Nationale pour la Recherche) project ”SIMDIM” (atomic scale simulations of dislocations in materials).

An application, to be sent by email to Joseph.Morillo@cemes.fr as a single pdf file, should include a cover letter, a resume, lists of publications and selected presentations as well as names and complete addresses of three referees. Applications will be considered until the position is filled.

Contact:

Prof. Joseph Morillo
CEMES-CNRS
29 rue Jeanne Marvig, BP 94347
31055 Toulouse Cedex 4
France

Email: Joseph.Morillo@cemes.fr

POSTDOCTORAL POSITIONS

Condensed Matter Theory Group
Department of Physics, Uppsala University, Sweden

Two postdoctoral positions in condensed matter theory group are available at the Department of Physics, Uppsala University, Sweden to work in the follwing research areas :

(1) Hydrogen Storage Materials
(2) Spintronics and Multiferroics
(3) Rechargeable lithium Batteries

All these projects will have a strong collaboration with experimental groups.

We are looking for candidates with PhD in physics/chemistry/materials science and experience in Density Functional calculations.

Interested candidates should submit their CV, two reference letters and the List of Publications, before **April 30, 2007** to Prof. Rajeev Ahuja, Department of Physics, Uppsala University, Box 530, 751 21 Uppsala, Sweden, e-mail: rajeev@fysik.uu.se .

Postdoctoral Position
RMIT University, Melbourne, Australia

A two year postdoctoral position is available to study self assembly of nanostructures on surfaces using the Kinetic Monte Carlo and Accelerated Molecular Dynamics Methods with Assoc. Prof. Salvy Russo and Prof. Ian Snook. The position is funded by an Australian Research Council Discovery Grant and is located in Applied Physics, School of Applied Sciences, RMIT University, Melbourne, Australia. The candidate will need experience in advanced theoretical and computational methods and the complexity of the work requires researchers at the post-doctoral level and a PhD in Computational/Theoretical Chemistry or Physics is required. Experience in the Kinetic Monte Carlo and/or Accelerated Molecular Dynamics Methods is desirable. Salary range is from $(AUS)58, 500to64$,300. Relocation expenses are available for applicants outside of Melbourne. For further information of this position or to apply please contact Assoc. Professor Salvy Russo salvy.russo@rmit.edu.au , Applied Physics, School of Applied Sciences, RMIT University, GPO Box 2476V, Melbourne, Victoria, Australia, 3001. Closing date Friday 4th May, 2007

Tenured Academic Staff

NANO Centre of Excellence
Department of Physics, Faculty of Science, University of Antwerp, Belgium

The University of Antwerp is a knowledge centre with 3,400 co-workers that performs ground-breaking and innovative research of international standing. The university takes special care to ensure optimal support and supervision of students, and pays constant attention to educational innovation. The university is an autonomous pluralistic institution that is committed to the enhancement of an open, democratic and multicultural society, and it pursues an equal opportunities policy.

The university is seeking to fill the following full-time vacancy (m/f) of tenured academic staff at the NANO Centre of Excellence, Department of Physics, Faculty of Science.

Job description: You will independently work within the NANO centre of excellence; in close collaboration however with the work performed at EMAT (emat.ua.ac.be) and CMT (cmt.ua.ac.be), you can be either an experimentalist or a theoretician, you will obtain national and international research funds, participate in networks, and supervise doctoral students, in accordance with your expertise, you will be involved in teaching the Bachelor or Master's students in Physics and/or Chemistry, as well as in supervising Master's and Doctoral theses students.

Profile and requirements: You hold a doctoral degree in science (physics, chemistry, materials science) you have an outstanding international scientific CV and at least 6 years of research experience in solid state physics, solid state chemistry of materials science, your academic achievements are situated within the top 10% of the broader field of study, preferably you also have experience in several forms of education in Bachelor's and/or Master's study programs, as well as experience in supervising doctoral students, ideally you should be at the bridge between EMAT and CMT.

We offer: A full time position as 'docent' (= level of lecturer) or higher, in agreement with your experience and your academic qualifications, the appointment is initially for a period of three years, after which it can become tenured depending on a favourable evaluation. The expected date of appointment is October 1st, 2007.

Interested?

Please fill out the mandatory application form (see

http://www.ua.ac.be/personeelsdienst

`http://www.ua.ac.be/main.aspx?c=*VACATURES&n=20319`

or call +32 (0)3 265 31 54) and send it to the University of Antwerp, Campus Middelheim, Personnel Department (cel AP), Middelheimlaan 1, BE-2020 Antwerpen, Belgium, at the latest on April 28th, 2007.

Information on the job description can also be obtained from the NANO Centre of Excellence Prof. G. Van Tendeloo (staf.vantendeloo@ua.ac.be) or from the head of the departement of Physics, Prof. F. Peeters (francois.peeters@ua.ac.be).

Specific questions on the administrative aspects of the job can be obtained from the department "Research", Dr. E. Spruyt (eric.spruyt@ua.ac.be).

Ph. D. Position

Theoretical simulation of Semiconductor-Biomolecule Hybrid Nanostructures

BCCMS, Bremen, Germany

A PhD scholarship is immediately available at the Bremen Center for Computational Materials Science (BCCMS) in Bremen. The successfull candidate will use a combination of molecular dynamics simulations, tight-binding and first-principles density-functional techniques to investigate chemical and physical interactions between semiconductor nanowires and biomolecules for molecular electronic device applications. The project is part of a cooperative research program between Germany and Israel. The research work is of a highly multidisciplinary nature and will be performed in close collaboration with experimental groups. For this position a solid background in theoretical solid state physics, materials science or theoretical chemistry is required. Existing expertise in electronic structure methods and atomistic modelling of materials will be considered as an advantage. Previous experience in scientific programming (Fortran or C) is highly appreciated. The BCCMS is part of an international network of research institutes and has worldwide collaborations, so that good English communication skills are essential.

In order to increase the percentage of female faculty members, female candidates with equal qualification will be given preference. The appointment will be for three years. Applications will be accepted until the position is filled.

Candidates should send their application including a cover letter indicating their motivation to apply for this position, a curriculum vitae, a list of publications, a statement about current research activities (preferably in pdf format) to: farchmin@bccms.uni-bremen.de

Contact and further information:

Prof. Thomas Frauenheim
email: thomas.frauenheim@bccms.uni-bremen.de
Dr. Andreia Luisa da Rosa
email: darosa@bccms.uni-bremen.de

Bremen Center for Computational Materials Science
Universität Bremen
Otto-Hahn-Allee, NW1/FB1
28359 Bremen, Germany

Postdoctoral Research Position
Hunter College, City University of New York

There is an immediate opening for a postdoctoral researcher in my group at Hunter College of CUNY (City University of New York). The group (PI Neepa Maitra) conducts research in functional development in time-dependent density functional theory, for use in chemistry and in strong-field physics. Experience in density functional theory methods is desirable, although not necessary. This position could be suitable for a person with a Ph. D. in either chemistry or physics.

Interested parties should send a CV electronically to

nmaitra@hunter.cuny.edu

and have three letters of recommendation emailed there.

If preferred, you may send the materials by mail to:

Neepa Maitra
Assistant Professor
Department of Physics and Astronomy
Hunter College & City University of New York
New York, NY 10021, USA

Phone: 212-650-3518
Fax: 212-772-5390
E-mail: nmaitra@hunter.cuny.edu

http://www.ph.hunter.cuny.edu/faculty/Maitra/neepa.html

Applications will be considered immediately and continue until the position is filled.

Postdoctoral Position(s) in Computational Materials Physics

Department of Physics and Astronomy, Rutgers University, USA

One or more postdoctoral positions in computational materials physics, under the supervision of Profs. David Vanderbilt, David Langreth and/or Karin Rabe, are expected to become available beginning in fall 2007. Experience with density-functional-based methods is strongly advantageous. Interested applicants should send a CV, including names and contact information for three references, to Prof. Rabe, preferably by May 1, 2007. Email submission in the form of a postscript or pdf file is preferred.

Prof. Karin Rabe
rabe@physics.rutgers.edu
Dept. of Physics and Astronomy
Rutgers University
136 Frelinghuysen Road
Piscataway, NJ 08854-8019
USA
Fax: 1-732-445-4400

POST-DOC POSITION AT POLITECNICO OF TORINO, ITALY

A postdoctoral position is available at the Physics Department of Politecnico di Torino (Italy) in the field of ab initio simulations of structural and electronic properties of nanostructured materials. The position will be open in May 2007 and will be funded for 3 years.

This post-doc position is funded by the Nano-Sci ERA (Nanoscience in the European Research Area) Consortium and it is part of a European research project involving four different research groups across Europe. The scope of the project is to devise new nanoscale architectures (coaxial-nanowires cNW) able to mimic the processes by which the photosynthetic organism harvest sunlight and convert its energy into chemo/electrical form. The successful candidate will use ab intio simulations to study the structural and electronic properties of semiconductor nanowires. In parallel, structural, optical and electrical characterization on the single cNW will be performed by the experimental groups involved in the project.

The candidate should hold a Ph.D. in physics, chemistry or materials science and should have previous experience with first-principles methods as well as scientific programming. A strong motivation to direct interaction with the experimental groups is also necessary.

The application to this position together with a résumé of recent research, a list of publications, and the names and emails of at least two referees should be sent by email to Giancarlo Cicero (email: giancarlo.cicero@polito.it) and Alessandra Catellani (email: catellani@imem.cnr.it).

Postdoctoral Position in the Theory of Condensed Matter Napoli University, Italy

The CNR-INFM Science Reseach Centre ’Coherentia’ at the Physics Department of Universitá di Napoli ’Federico II’ opens a postodoctoral position founded by the Euro Science Foundation (ESF) collaborative project ’Fundamental of Nanoelectronics (FONE): SPINTRA’

(http://www.ifmpan.poznan.pl/spintra/)

under the supervision of Prof. A. Tagliacozzo. Focus will be on spin states and transport in quantum dots, rings and Hall bars with spin-orbit interaction as well as coherent transport in hybrid mesoscopic superconductor/semiconductor systems.

Applicants should hold or be close to acquiring a Ph. D. in Theoretical Condensed Matter Physics, or a related field. Computational experience or training in field theory methods will be welcome. The post will be for one year with a possible extension of one more year. The salary of the succesful candidate will start with 21000 EUR with some dependence on the experience.

Initial deadline for applications is June 2007 the 15th, but the starting date for the post is flexible within year 2007 (better before 30th of September). Anyhow the search will be continued until the post is filled .

Interested candidates may contact Arturo Tagliacozzo directly (arturo@na.infn.it).

`http://people.na.infn.it/~arturo/group/mesoscopic_group.html`

Ph. D. Studentships at Imperial College London, U. K.

Two 3-year studentships are available immediately in the Department of Materials at Imperial College for application of ab initio methods to support

1) the design of high-temperature shape-memory alloys and

2) the design of high-performance cathodes for solid-oxide fuel-cells.

A strong theoretical background in quantum mechanics, statistical mechanics and solid state theory will be required, together with good computational skills and an interest in applications. If you are interested in one or both, please send a CV, covering letter and the names of two referees to the address below.

Professor M. W. Finnis
Department of Materials
and Department of Physics
Imperial College London
Exhibition Road
London SW7 2AZ
U. K.
Email: m.finnis@ic.ac.uk
Tel: +44 (0) 207 59 46812
Fax: +44 (0) 207 59 46757

Research Associate in Condensed Matter Theory

Department of Physics and Astronomy

Nebraska Center for Materials and Nanoscience
University of Nebraska-Lincoln, Lincoln, NE

Applications are invited for a research associate position in computational materials science to conduct research in theory of electronic and transport properties of magnetic, ferroelectric and multiferroic nanostructures. This project is funded jointly by the Nanoelectronics Research Corporation (NRI) and National Science Foundation (NSF) and is closely linked to experimental studies being performed by the industrial companies involved in the NRI and the NSF-funded Materials Research Science and Engineering Center at the University of Nebraska. We are seeking for a highly motivated researcher with experience in computational materials science who will join an active theoretical group and will participate in multidisciplinary research projects concerned with magnetoelectric properties of ferromagnetic-ferroelectric interfaces, electron and spin transport in ferroelectric and multiferroic junctions and switching behavior in all-oxide heterostructures. Required qualifications are

(i) PhD in physics or closely related field;
(ii) strong research accomplishments in condensed matter/materials science theory;
(iii) expertise in electronic band structure calculations such as LMTO, FLAPW, and/or VASP.

The appointment is initially for one year with the possibility of renewal for up to three years. Salary is commensurate with qualifications and experience. Screening of applications will begin immediately and continue until a suitable candidate is found. Applicants should send a letter of application, curriculum vitae, list of publications, and contact information for at least two references to Evgeny Tsymbal at tsymbal@unl.edu.

Evgeny Y. Tsymbal
Professor of Physics
University of Nebraska-Lincoln
Department of Physics and Astronomy
213E Ferguson
Lincoln, NE 68588-0111

Phone: (402) 472 2586
Fax: (402) 472 2879
E-mail: tsymbal@unl.edu

Web: `http://physics.unl.edu/~tsymbal/tsymbal.html`

Postdoctoral Position in Computational Solid State Physics
University of Nebraska-Lincoln, U. S. A.

A postdoctoral position in computational solid state physics is available in the group of Prof. Kirill Belashchenko at the University of Nebraska-Lincoln. The successful applicant will be involved in the studies of magnetism and transport in materials and heterostructures using density-functional electronic structure theory. The initial appointment will be for one year with a possible extension upon mutual agreement. Candidates must have a doctoral degree in physics and experience in electronic structure calculations. Desirable qualifications include strong motivation, experience in the studies of magnetic materials and/or electronic transport, and scientific programming skills. Interested candidates should send an application letter, detailed CV, list of publications, and contact information for at least two references to Kirill Belashchenko by email (preferably in PDF format).

Review of applications is in progress and will continue until the position is filled.

UNL is committed to a pluralistic campus community through EEO/AA. We assure reasonable accommodation under ADA/504; contact Beth Farleigh at (402)472-2770 for assistance.

Kirill Belashchenko
Assistant Professor
Department of Physics and Astronomy
University of Nebraska-Lincoln
Lincoln, NE 68588-0111, USA
Phone: (402)472-2396
Fax: (402)472-2879
Email: kdbel@unlserve.unl.edu

Postdoctoral Positions on the Theory of Thermal and Thermoelectric Transport

C.E.A., Grenoble, France

The Laboratory for New Energy Technologies and Nanomaterials (LITEN), of the French Atomic Energy Commission (CEA), in Grenoble, France is looking for talented individuals whose expertise and interests can contribute to the theoretical and computational investigation of thermal, electronic, and thermoelectric transport through nanostructured materials and/or nanoscale devices. The theoretical research will be conducted in parallel with experimental work carried out at LITEN and several other laboratories in the U.S. and France.

A PhD in Physics, Materials Science, Electrical Engineering, Mechanical Engineering, or related field, is required. Experience in one or more of the following areas is a plus: theory of thermal, electronic, or thermoelectric transport; molecular dynamics; ab- initio methods for materials properties; Boltzmann transport equation techniques; radiative heat transfer; Monte Carlo methods applied to thermal transport; Non-Equilibrium Greens Functions.

Interested candidates should send their resume, publication list, and contact information for at least three references, electronically to the group lead, Dr. Natalio Mingo, e-mail: natalio.mingo@cea.fr . Applications will be accepted until position is filled.

CNRS Postdoctoral Position in Paris

(24 months, starting date: September or October 2007)

Project: Superconductivity of doped/intercalated carbon nanotubes and graphite

Details: We are looking for a theoretical postdoc to study, with density-functional-theory, the structural, vibrational and electronic properties of graphite and carbon nanotubes, intercalated by donor/acceptor atom and/or molecules. We aim to improve the superconducting properties of intercalated graphite, and to obtain similar or better properties in intercalated carbon nanotube bundles. The superconductivity of Ca-intercalated graphite (CaC_6) with a critical temperature of 11.5 K at room pressure and of 15.1 K under pressure was recently measured in our laboratory. These temperatures are the highest ever observed in this kind of systems. Our theoretical group explained the occurrence of superconductivity in CaC_6. In addition we also published several papers on the vibrational properties and electron-phonon coupling of graphite, carbon nanotubes, and graphene (see list below).

Required skills: The candidate must be familiar with quantum theory of solid state and with ab initio methods based on density functional theory. A strong motivation to direct interaction with the experimental groups is also necessary

Some of our recent works on MgB_2, graphite and NTs: PRL 90, 095506 (2003); PRL 93, 185503 (2004); PRL 95, 087003 (2005); PRL 97, 266407 (2006); PRL 97, 187401 (2006); PRL 98, 067002 (2007); Nature Materials 5, 3 (2007). PRB 68, 220509(R) (2003); PRB 71, 064501 (2005); PRB B 73, 155426 (2006); PRB 73, 155426 (2006); PRB 75, (March 2007) cond-mat/0702493.

The interested candidates should send an email with a CV and the names and contact information of at least two references to: mauri@impmc.jussieu.fr and marco.saitta@impmc.jussieu.fr

Laboratory web address: www.impmc.jussieu.fr

- Prof. Francesco Mauri

Institut de Minéralogie et de Physique des Milieux Condensés
Universit Pierre et Marie Curie
Campus Boucicaut, 140 rue de Lourmel
75015 Paris, France

Office location: bat. 7, 1ere etage, porte 9
Email: Francesco.Mauri@impmc.jussieu.fr

Tel: 33-1-44272764
Fax: 33-1-44273785

C2C Postdoctoral Fellowship in Cracow (Poland)

As part of the Marie Curie Research Training Network c2c project the Institute of Nuclear Physics, PAN, Cracow, Poland, (Department Materials Research by Computers, MRC,

http://wolf.ifj.edu.pl/depX/)

invites applications for

ONE POSTDOC FELLOWSHIP FOR ONE YEAR

with a possible extension for a second year at one of the other Network partners.

Within c2c the team at the MRC will focus on mechanical, elastic and thermodynamical properties of minerals. The c2c projects at the MRC will investigate, using ab initio computational techniques, the high-pressure properties of major slab and mantle minerals, with a special interest on mechanical properties and P-V-T equation of state in order to determine the strength, density and buoyancy of subducting crust. The effect of chemical composition, phase transitions, water content, partial melting, etc., will be investigated.

The MRC have extensive expertise in high pressure and temperature ab initio calculations in the field of mineral physics. We host computational tools for our research as well as have full access to national supercomputing facilities. We also have a full set of software tools at our disposal. The research work will involve the cooperation with other nodes of the c2c network - particularly Bayerisches Geoinstitut at the University of Bayreuth, Germany

(http://www.bgi-uni.bayreath.de/)

and University College London, United Kingdom.

The successful candidate should ideally have experience in computational simulations. Applicants should send a curriculum vitae, list of publications and a summary of research interests to either the project coordinator (c2c@uni-bayreath.de), or the partner at MRC (Dr Pawel T. Jochym, Pawel.Jochym@ifj.edu.pl) or Prof. Krzysztof Parlinski, Krzysztof.Parlinski@ifj.edu.pl).

Prof. dr hab. Krzysztof Parlinski
Institute of Nuclear Physics
Polish Academy of Sciences
ul.Radzikowskiego 152, 31-342 Cracow
Poland
E-mail: krzysztof.parlinski@ifj.edu.pl
http://wolf.ifj.edu.pl/deptX/

C2C Ph. D. Fellowship, Cracow (Poland)

As part of the Marie Curie Research Training Network c2c project the Institute of Nuclear Physics, PAN, Cracow, Poland, (Department Materials Research by Computers, MRC, http://wolf.ifj.edu.pl/depX/) invites applications for

ONE Ph. D. FELLOWSHIP FOR ONE YEAR

with expected extension for TWO MORE YEARS.

The c2c projects at the MRC will investigate, using ab initio computational techniques, the high-pressure properties of major slab and mantle minerals, with a special interest on mechanical properties and P-V-T equation of state in order to determine the strength, density and buoyancy of subducting crust. The effect of chemical composition, phase transitions, water content, partial melting, etc., will be investigated.

The work will be mainly performed at the MRC in Cracow. Visits to other nodes of the network will be possible. The MRC have extensive expertise in high pressure and temperature ab initio calculations in the field of mineral physics. We host computational tools for our research as well as have full access to national supercomputing facilities. We also have a full set of software tools at our disposal. The research work will involve the cooperation with other nodes of the c2c network - particularly Bayerisches Geoinstitut at the University of Bayreuth

(http://www.bgi-uni.bayreath.de/),

Germany and University College London, United Kingdom.

The successful candidate should preferably have a background in Physics or Material Sciences or Earth Sciences. Applicants should send a curriculum vitae, list of publication, and a summary of research interests in a single pdf file to the project coordinator (c2c@uni-bayreath.de), or the partner at MRC (Dr Pawel T. Jochym, Pawel.Jochym@ifj.edu.pl) or Prof. Krzysztof Parlinski, Krzysztof.Parlinski@ifj.edu.pl).

Prof. dr hab. Krzysztof Parlinski
Institute of Nuclear Physics
Polish Academy of Sciences
ul.Radzikowskiego 152, 31-342 Cracow
Poland
E-mail: krzysztof.parlinski@ifj.edu.pl
http://wolf.ifj.edu.pl/deptX/

Postdoctoral Position in First-Principles Based Modeling of Alloys for Nuclear Applications
University of Wisconsin, Madison, USA

A postdoctoral position is available immediately in the group of Dane Morgan in the Department of Materials Science and Engineering at University of Wisconsin, Madison. The research will be in the general area of combining First-Principles (DFT) and standard and kinetic Monte Carlo methods to model thermodynamics, diffusion, and evolution of radiation damage in multicomponent alloys of interest for nuclear applications. Familiarity with DFT methods and alloy thermodynamic and kinetic modeling is essential. The appointment is initially for one year with possible extension. Interested applicants should send CV (preferably in PDF format) and contact information for 3 references to Dane Morgan at ddmorgan@wisc.edu. Consideration of candidates will begin immediately and will continue until the position is filled.

Dane Morgan Assistant Professor
244 Materials Science & Engineering
1509 University Avenue
Madison, WI 53706-1595
Phone: 608-265-5879
Fax (department): 608-262-835
Email: ddmorgan@wisc.ed
Web: `http://www.engr.wisc.edu/mse/faculty/morgan_dane.html`

7 Abstracts

Optical properties of dilute nitrogen GaInNAs quantum dots

Stanko Tomić
Computational Science and Engineering Department, CCLRC Daresbury Laboratory, Warrington, Cheshire WA4 4AD, United Kingdom

Abstract

We present a theoretical study of the ground state optical transition matrix element in quantum dots (QD) with a dilute amount of nitrogen. We have investigated the interplay between the nitrogen to the conduction band mixing, and piezoelectric field on the optical matrix element. With a reduced amount of indium and an increased amount of nitrogen in the QD the optical matrix element becomes on the average larger and less sensitive to the variation of both the QD shape and size than is the case of an InNAs QD. The optical characteristics at room temperature and 1.5 μm wavelength are discussed.

(Submitted to Appl. Phys Lett.)
Contact person: s.tomic@dl.ac.uk

Studying spintronics materials with soft x-ray resonant scattering

Gerrit van der Laan
Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK

Abstract

Soft x-ray resonant magnetic scattering offers a unique element-, site- and valence- specific probe to study magnetic structures on a length scale from 1 to 1000 nm. This new technique, which combines x-ray scattering with x-ray magnetic circular and linear dichroism, is ideally suited to investigate magnetic superlattices and magnetic stripe domains. Recent results that are presented here include element-specific magnetic studies on interfaces, thin films, magnetic multilayers, self-organising magnetic domain structures, magnetic layer profiles, patterned samples, and magnetic nano-objects using coherent x-rays. Soft x-ray diffraction to study the interplay between charge, spin and orbital ordering in correlated $3d$ transition metal systems, such as manganites, is also discussed.

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Manuscript available from g.vanderlaan@dl.ac.uk.

Heusler alloy/semiconductor hybrid structures

A. Hirohata
Frontier Research System, RIKEN, 2-1 Hirosawa, Wako, Japan
M. Kikuchi
Department of Materials Science, Graduate School of Engineering,
ıTohoku University, Sendai, Japan
N. Tezuka and K. Inomata
CREST, Japan Science and Technology Agency, Honcho, Kawaguchi, Japan
J.S. Claydon and Y.B. Xu
Department of Electronics, University of York, Heslington, York YO10 5DD, UK
G. van der Laan
Magnetic Spectroscopy, Daresbury Laboratory, Warrington WA4 4AD, UK

Abstract

Heusler alloys are theoretically predicted to become half-metals at room temperature (RT). The advantages of using these alloys are good lattice matching with III-V semiconductors, high Curie temperature above RT and intermetallic controllability for spin density of states at the Fermi level. These alloys are categorized into half and full Heusler alloys dependent upon the crystalline structures, each of which is discussed both experimentally and theoretically in Sections 2 and 3, respectively. As an example, our recent studies on epitaxial $L2_1$ $Co_2Cr_{1-x}Fe_xAl(0\ 0\ 1)/GaAs(0\ 0\ 1)$ hybrid structures are presented here. Both structural and magnetic characterizations on an atomic scale are typically carried out in order to prove the half-metallicity at RT as described in Section 4. Atomic ordering in the Heusler films is directly observed by X-ray diffraction and is also indirectly measured by the temperature dependence of electrical resistivity. Element specific magnetic moments and spin polarization of the Heusler alloy films are directly estimated by using X-ray magnetic circular dichroism and Andreev reflection, respectively. By employing these alloy films into a spintronic device, diffusive spin-polarized electron transport may offer highly efficient spin injection across a direct interface between the Heusler alloy film and the semiconductor, while ballistic transport in a magnetic tunnel junction may further improve areal density of a magnetic random access memory with a large magnetoresistance ratio at RT as discussed in Section 5. A brief summary is provided at the end of this review.

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Spatial distribution and magnetism in poly-Cr doped GaN from first-principles

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Abstract

Large scale density-functional theory calculations have been performed to understand the spatial distribution and magnetic coupling of Cr doped GaN, in which exhaustive structural and magnetic configurations have been investigated by doping of up to 5 Cr atoms in large supercells. Our results provide direct evidence that the distribution of the doped magnetic ions is neither homogenous nor random as widely assumed previously. Rather, under both Ga-rich and N-rich growth conditions, the Cr atoms have a strong tendency to form substitutional, embedded clusters with short-range magnetic interactions maintaining the wurtzite structure. Significantly, while the ferromagnetic state is favored for pair-doping, for more than 2-Cr-atom clustering configurations, states containing antiferromagnetic or ferrimagnetic coupling with net spins in the range of 0.06∼1.47 μ_B/Cr are preferred. The formation of embedded clusters leads to notable local structural distortions and considerable magnetic moments on the Cr-bonded N atoms. Also importantly, the electrical properties (metallic, half-metallic, or semiconducting) are found to strongly depend on the dopant concentration. We propose a picture where various cluster configurations coexist and the statistical distribution and associated magnetism depend sensitively on sample growth details. The results obtained are in agreement with recent experiments.Such a view can explain many hitherto puzzling experimental observations – e.g., the much lower value of the measured mean saturation magnetic moment on Cr as compared to the theoretically predicted value for the isolated dopants; the anomalous lattice constant change in relation to the dopant concentration and temperature; and the strong dependence of the magnetization on the Cr concentration, growth temperature and annealing. We find a similar behavior for Mn in GaN, and Cr and Mn in AlN, and argue that such a scenario may also hold for other dilute magnetic semiconductor systems.

(Physical Review B, in press)
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An efficient virtual crystal approximation capable of treating heterovalent atoms; applied to (1-x)$BiScO_3$–x$PbTiO_3$

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Abstract

It is well accepted that the virtual crystal approximation (VCA) is an effective method to study solid solutions and alloys with first principles. Here we propose an another approach based on a well designed averaging of the pseudo wavefunctions. Due to the fact that under physical and numerical considerations there is a subtle arbitrariness in constructing the Kleinman-Bylander (KB) pseudopotential, we can construct the orthonormalized pseudo wavefunctions as well as pseudo potentials of the virtual atom in the manner of averaging. It is proved that this extended averaging approach can provide the reasonable properties of the heterovalent solid solutions, together with the advantege of very simplicity. Our results for the perovskite ferroelectrics, (1-x)$BiScO_3$–x$PbTiO_3$, satisfies well the Vegard's law with respect to the cubic lattice constants and displays improved values with respect to the structural, electronic, electrical and elastic properties, compared with the preveous work (Íñiguez, Vanderbilt and Bellaiche 2003 Phys. Rev. B **67** 224107).

Journal of Physics: Condensed Matter

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Representing molecule-surface interactions with symmetry-adapted neural networks

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Abstract

The accurate description of molecule-surface interactions requires a detailed knowledge of the underlying potential-energy surface (PES). Recently, neural networks (NNs) have been shown to be an efficient technique to accurately interpolate the PES information provided for a set of molecular configurations, e.g. by first-principles calculations. Here, we further develop this approach by building the NN on a new type of symmetry functions, which allows to take the symmetry of the surface exactly into account. The accuracy and efficiency of such symmetry-adapted NNs is illustrated by the application to a six-dimensional PES describing the interaction of oxygen molecules with the Al(111) surface.

(submitted to: Journal of Chemical Physics)
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Towards an exact treatment of exchange and correlation in materials: Application to the "CO adsorption puzzle" and other systems

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Abstract

It is shown that the errors of present-day exchange-correlation (xc) functionals are rather short ranged. For extended systems the *correction* can therefore be evaluated by analyzing properly chosen clusters and employing highest-quality quantum chemistry methods. The xc *correction* rapidly approaches a universal dependence with cluster size, exhibiting a simple analytical behavior. The method is applicable to bulk systems as well as to defects in the bulk and at surfaces. It is demonstrated here for CO adsorption at transition-metal surfaces, where present xc functionals dramatically fail to predict the correct adsorption site, and for the crystal bulk cohesive energy.

(Phys. Rev. Lett (accepted))
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CO oxidation at Pd(100): A first-principles *constrained* thermodynamics study

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Abstract

The possible formation of oxides or thin oxide films (surface oxides) on late transition metal surfaces is recently being recognized as an essential ingredient when aiming to understand catalytic oxidation reactions under technologically relevant gas phase conditions. Using the CO oxidation at Pd(100) as example, we investigate the composition and structure of this model catalyst surface over a wide range of (T, p)-conditions within a multiscale modeling approach where density-functional theory is linked to thermodynamics. The results show that under the catalytically most relevant gas phase conditions a thin surface oxide is the most stable "phase" and that the system is actually very close to a transition between this oxidic state and a reduced state in form of a CO covered Pd(100) surface.

(submitted to: Phys. Rev. B)
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Elastic Response of Cubic Crystals to Biaxial Strain: Analytic Results and Comparison to Density Functional Theory for InAs

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Abstract

The elastic energy of a biaxially strained material depends on both the magnitude and the plane of the applied biaxial strain, and the elastic properties of the material. We employ continuum-elasticity theory (CET) to determine general analytic expressions for the strain tensor, the Poisson ratio, and the elastic energy for materials with cubic crystal symmetry exposed to biaxial strain in arbitrary planes. In application to thin homogeneously strained films on a substrate, these results enable us to estimate the role of elastic energy for any substrate orientation. When calculating the elastic response to biaxial strain in an arbitrary plane by numerical methods, our analytic results make it possible to set up these calculations in a much more efficient way. This is demonstrated by density-functional theory (DFT) calculations of the Poisson ratio and elastic energy upon biaxial strain in several planes for the case of InAs. The results are in good agreement with those of CET, but show additional non-linear contributions already at moderate biaxial strain.

(submitted to: Phys. Rev. B)
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First principles free energy analysis of helix formation: The origin of the low entropy in π-helices

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Abstract

The free energy change arising from the folding of a fully extended structure (FES) of the infinite poly-L-alanine chain into various helical conformations, including the α-, π-, and 3_{10}-helix, was calculated by employing DFT-GGA and the harmonic approximation. Our results show that the vibrational entropy strongly reduces the stability of the helical conformations with respect to the FES. However, for α- and 3_{10}-helices, the enthalpic contributions arising from hydrogen bonds are sufficiently strong to maintain their stability even above room temperature. In contrast, the π- helix shows a more pronounced temperature dependence than the α- or 3_{10}-helix, making it unstable with respect to the FES above room temperature. The latter trend is shown to be a generic behavior of the π-helix conformation, i.e., independent of the specific amino acid sequence.

(submitted to: Phys. Rev. Lett.)
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Vertex corrections in localized and extended systems

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Abstract

Within many-body perturbation theory we apply vertex corrections to various closed-shell atoms and to jellium, using a local approximation for the vertex consistent with starting the many-body perturbation theory from a DFT-LDA Green's function. The vertex appears in two places – in the screened Coulomb interaction, W, and in the self-energy, Σ – and we obtain a systematic discrimination of these two effects by turning the vertex in Σ on and off. We also make comparisons to standard GW results within the usual random-phase approximation (RPA), which omits the vertex from both. When a vertex is included for closed-shell atoms, both ground-state and excited-state properties demonstrate only limited improvements over standard GW. For jellium we observe marked improvement in the quasiparticle band width when the vertex is included only in W, whereas turning on the vertex in Σ leads to an unphysical quasiparticle dispersion and work function. A simple analysis suggests why implementation of the vertex only in W is a valid way to improve quasiparticle energy calculations, while the vertex in Σ is unphysical, and points the way to development of improved vertices for *ab initio* electronic structure calculations.

(submitted to: Phys. Rev. B)
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Ultrathin oxides: bulk-oxide-like model surfaces or unique films?

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Abstract

To better understand the electronic and chemical properties of wide-gap oxide surfaces at the atomic scale, experimental work has focussed on epitaxial films on metal substrates. Recent findings show that these films are considerably thinner than previously thought. This raises doubts about the transferability of the results to surface properties of thicker films and bulk crystals. By means of density-functional theory and approximate quasiparticle energy corrections we demonstrate for three characteristic wide-gap oxides (silica, alumina, and hafnia) the influence of the substrate and highlight critical differences between the ultrathin films and surfaces of bulk materials. Our results imply that monolayer-thin oxide films have rather unique properties.

(submitted to: Phys. Rev. Lett.)
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Lanthanide contraction and magnetism in the heavy rare earth elements

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Abstract

The heavy rare earth elements crystallize into hexagonally close packed (h.c.p.) structures and share a common outer electronic configuration, differing only in the number of 4f electrons they have. These chemically inert 4f electrons set up localized magnetic moments, which are coupled via an indirect exchange interaction involving the conduction electrons. This leads to the formation of a wide variety of magnetic structures, the periodicities of which are often incommensurate with the underlying crystal lattice. Such incommensurate ordering is associated with a 'webbed' topology of the momentum space surface separating the occupied and unoccupied electron states (the Fermi surface). The shape of this surface, and hence the magnetic structure, for the heavy rare earth elements is known to depend on the ratio of the interplanar spacing c and the interatomic, intraplanar spacing a of the h.c.p. lattice. A theoretical understanding of this problem is, however, far from complete. Here, using gadolinium as a prototype for all the heavy rare earth elements, we generate a unified magnetic phase diagram, which unequivocally links the magnetic structures of the heavy rare earths to their lattice parameters. In addition to verifying the importance of the c/a ratio, we find that the atomic unit cell volume plays a separate, distinct role in determining the magnetic properties: we show that the trend from ferromagnetism to incommensurate ordering as atomic number increases is connected to the concomitant decrease in unit cell volume. This volume decrease occurs because of the so-called lanthanide contraction, where the addition of electrons to the poorly shielding 4f orbitals leads to an increase in effective nuclear charge and, correspondingly, a decrease in ionic radii.

(Nature **446**, 650-653 (2007))

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Oxygen Vacancies in Transition Metal and Rare Earth Oxides: Current state of understanding and remaining challenges

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Abstract

Defects at transition metal (TM) and rare earth (RE) oxide surfaces, neutral oxygen vacancies in particular, play a mayor role in a variety of technological applications. This is the motivation of numerous studies of partially reduced oxide surfaces. We review, discuss, and compare theoretical data for structural and electronic properties and energetic quantities related to the formation of oxygen defects at TM and RE oxide surfaces using TiO_2, ZrO_2, V_2O_5, and CeO_2 as examples. Bulk defects, as far as relevant for comparison with the properties of reduced surfaces, are briefly reviewed. Special attention is given to the fate of the electrons left in the system upon vacancy formation and the ability of state–of–the–art quantum–mechanical methods for providing reliable energies and an accurate description of the electronic structure of the partially reduced oxide systems.

(Surf. Sci. Rep., in press)
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Elastic constants and high-pressure structural transitions in lanthanum monochalcogenides from experiment and theory

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Abstract

The high-pressure structural behavior of lanthanum monochalcogenides is investigated by theory and experiment. Theory comprises density functional calculations of LaS, LaSe and LaTe with the general gradient approximation for exchange and correlation effects, as implemented within the full-potential linear muffin-tin orbital method. The experimental studies consist of high-pressure angle dispersive x-ray diffraction investigations of LaS and LaSe up to a maximum pressure of 41 GPa. A structural phase transition from the NaCl type to CsCl type crystal structure is found to occur in all cases. The experimental transition pressures are 27-28 GPa and 19 GPa, for LaS and LaSe, respectively, while the calculated transition pressures are 29 GPa, 21 GPa and 10 GPa for LaS, LaSe and LaTe, respectively. The calculated ground state properties such as equilibrium lattice constant, bulk modulus and its pressure derivative, and Debye temperatures are in good agreement with experimental results. Elastic constants are predicted from the calculations.

(submitted to Phys. Rev. B)
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High-pressure structural, elastic and electronic properties of the scintillator host material, $KMgF_3$

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Abstract

The high-pressure structural behaviour of the fluoroperovskite $KMgF_3$ is investigated by theory and experiment. Density functional calculations were performed within the local density approximation and the generalized gradient approximation for exchange and correlation effects, as implemented within the full-potential linear muffin-tin orbital method. *In situ* high-pressure powder x-ray diffraction experiments were performed up to a maximum pressure of 40 GPa using synchrotron radiation. We find that the cubic $Pm\bar{3}m$ crystal symmetry persists throughout the pressure range studied. The calculated ground state properties – the equilibrium lattice constant, bulk modulus and elastic constants – are in good agreement with experimental results. By analyzing the ratio between the bulk and shear modulii, we conclude that $KMgF_3$ is brittle in nature. Under ambient conditions, $KMgF_3$ is found to be an indirect gap insulator with the gap increasing under pressure.

(submitted to Phys. Rev. B)
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8 Presenting Other Initiatives

8.1 European Theoretical Spectroscopy Facility: First call for proposals

Deadline for submission: 11 April 2007

Initiative of the Nanoquanta Network of Excellence (http://www.nanoquanta.eu)

The European Theoretical Spectroscopy Facility is a professionally-managed ”knowledge centre” which aims to provide experimental and industrial researchers, among others, with easy and supported access to modern theory and simulation facilities for electronic excited states in matter, particularly nanostructures, as well as nanoelectronics and the energetics of atomic motion on the nanometre scale.

The ETSF's first call for proposals has now been published at ¡http://www.etsf.eu¿. I invite you to consider submitting a proposal, which is addressed to all potential ETSF users, including both experimental groups and theoreticians working in neighbouring fields, such as chemistry, biology, physics and medicine, from academia, research institutions or the private sector. Selection will be based on scientific interest and feasibility, and on the level of resources required.

In these pilot projects, the ETSF contribution to the projects will be entirely funded by the EU Nanoquanta Network of Excellence grant. Project proposals may be submitted through the web site from Monday, 12th March 2007 until 23:59 on Wednesday, 11th April 2007.

We hope that this opportunity will be of interest to you, and would be happy to answer any questions you may have about the call or the ETSF more generally.

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9 SCIENTIFIC HIGHLIGHT OF THE MONTH: Calculating Scattering Matrices by Wave Function Matching

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Calculating Scattering Matrices by Wave Function Matching

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Abstract

As devices are reduced in size, interfaces start to dominate electrical transport making it essential to be able to describe reliably how they transmit and reflect electrons. Wave function matching (WFM) is a transparent technique for calculating transmission and reflection matrices suitable for any Hamiltonian that can be represented in tight-binding form. A first-principles Kohn-Sham Hamiltonian represented on a localized orbital basis or on a real space grid has such a form. WFM is based upon direct matching of the scattering-region wave function to the Bloch modes of the leads. In this paper we give a pedagogical introduction to WFM. We briefly discuss WFM for calculating the conductance of atomic wires, using a real space grid implementation. A tight-binding muffin-tin orbital implementation very suitable for studying spin-dependent transport in layered magnetic materials is illustrated by looking at spin-dependent transmission through ideal and disordered interfaces.

1 Calculating the scattering matrix from first principles

Various methods have been developed for calculating the transmission of electrons through an interface (or a more extended scattering region) from first principles [1–15], or using as input electronic structures which were calculated from first principles [16–22]. Most are based upon a formulation for the conductance in terms of non-equilibrium Green's functions (NEGF) [23] which reduces in the appropriate limit to the well known Fisher-Lee linear-response form [24] for the conductance of a finite disordered wire embedded between crystalline leads. An alternative technique, suitable for Hamiltonians that can be represented in tight-binding form, has been formulated by Ando [25] and is based upon direct matching of the scattering-region wave function to the Bloch modes of the leads[1]. A third approach based upon "embedding" [28,29] has been combined with full-potential linearized augmented plane wave method to yield what is probably the most accurate scheme to date [11, 12] but is numerically very demanding.

Our main purpose is to outline a scheme suitable for studying microscopic transport in the linear response regime in inhomogeneous, mainly layered, materials which is physically transparent and first-principles, i.e., requiring no free parameters. Landauer and Büttiker formulated the problem of electronic transport in terms of scattering matrices where the transmission matrix element $t_{n,m}$ is the probability amplitude that a state $|n\rangle$ in the left-hand lead incident on the scattering region from the left (see Fig. 1) is scattered into a state $|m\rangle$ in the right-hand lead. The conductance $G = dI/dV|_{V=0}$ in the linear response regime is given by

$$G = \frac{e^2}{h} \sum_{n,m} |t_{n,m}|^2. \tag{1}$$

The Landauer-Büttiker approach is intuitively very appealing because wave transport through interfaces is so naturally described in terms of transmission and reflection. Usually, explicit calculation of the scattering states is avoided by making use of the invariance properties of the trace in Eq. 1 to calculate the conductance directly from Green functions expressed in some convenient localized orbital representation [23]. However, we want to make contact with the large body of theoretical literature on mesoscopic physics [30, 31] which requires calculation of the full microscopic transmission and reflection matrices and make use of the explicit knowledge of the scattering states to analyze our numerical results. Our requirement of physical transparency is satisfied by choosing a computational scheme which yields the full scattering matrix and not just the conductance.

Any workable first-principles scheme is at present based upon an independent particle approximation. An extremely successful framework for calculating ground state properties of a wide variety of materials is Density Functional Theory (DFT) using functionals based upon the Local Density Approximation (LDA) or the Generalized Gradient Approximation (GGA). DFT/LDA or GGA calculations and their spin-polarized versions yield a charge (spin) density in all space as well as a Kohn-Sham effective potential. We assume that the latter can be used in describing the electron transport within the Landauer-Büttiker formalism in the linear response regime. This then satisfies our requirement of introducing no free parameters.

To calculate transmission and reflection matrices from first principles, we combined the wave-function matching (WFM) formalism described by Ando [25] for an empirical tight-binding Hamiltonian, with an ab-initio tight-binding Hamiltonian. A version of this method has been implemented for a real-space grid, using a high order finite difference scheme. It has been applied to the calculation of the conductance of atomic wires [15, 32]. Another implementation is based upon a representation on an ab-initio TB-MTO basis [7,33,34]. The method which results, was applied to a number of problems of current interest in spin-transport: to the calculation of spin-dependent interface resistances where interface disorder was modeled by means of large lateral supercells [7,35]; to the first principles calculation of the spin mixing conductance parameter entering theories with non-collinear magnetizations, relevant for the spin-transfer torque [36] and the related problem of Gilbert damping enhancement in the presence of interfaces [37]; to a generalized scattering formulation of the suppression of Andreev scattering at a ferromagnetic|superconducting interface [38]; to the problem of how spin-dependent interface resistances influence spin injection from a metallic ferromagnet into a III–V semiconductor [39–41] and to the influence of roughness and disorder on tunneling magnetoresistance [42].

In this section we give a general exposé of the wave-function matching method. In Sec. 2 we will discuss an application to atomic wires based upon a real space grid implementation. Applications to (magnetic)

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[1] The relationship between the wave function matching (WFM) [25] and Green function [23, 24] approaches is not immediately obvious. It was suggested recently that WFM was incomplete [26] but the complete equivalence of the two approaches could be proven [27].

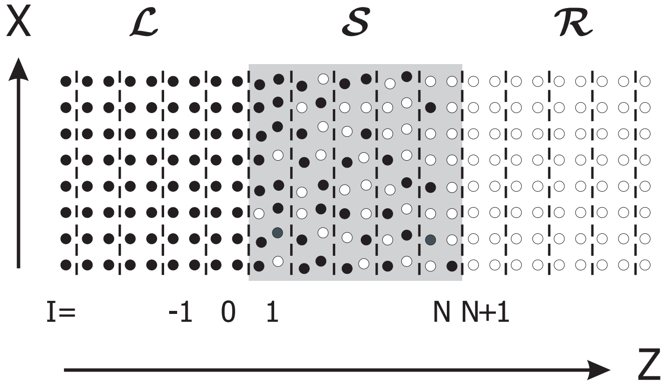

Figure 1: Sketch of the configuration used in the Landauer-Büttiker transport formulation to calculate the two terminal conductance. A (shaded) scattering region ($\mathcal{S}$) is sandwiched by left- ($\mathcal{L}$) and right-hand ($\mathcal{R}$) leads which have translational symmetry and are partitioned into principal layers perpendicular to the transport direction. The scattering region contains N principal layers but the structure and chemical composition are in principle arbitrary.

interfaces based upon a TB-MTO implementation are discussed in Sec. 3.

1.1 Formalism

In layered structures Bloch translational symmetry is broken so that the Kohn-Sham equations have to be solved for the infinite system represented by Fig. 1. This problem is reduced to finite size by replacing the semi-infinite leads by appropriate energy dependent boundary conditions as represented by Fig. 2. This can be achieved by the wave-function matching (WFM) method for calculating the transmission and reflection matrices due to Ando [25]. In the next sections we will give a very simple, pedagogical introduction to this method. We restrict ourselves to the linear response regime. The full details of the formalism and of the implementations can be found in Refs. [15, 27, 34]

1.1.1 Wave function matching in one dimension

The essence of WFM can be explained at an introductory quantum mechanics level. We start from Fig. 3, which represents a one-dimensional potential barrier with constant potentials in the leads (the left and right regions). We discretize the Schrödinger equation and approximate the second derivative by a first order finite difference expression.

$$E\psi_i + \frac{\hbar^2}{2m}\left\{\frac{(\psi_{i+1}-\psi_i)-(\psi_i-\psi_{i-1})}{\Delta^2}\right\} - V_i\psi_i = 0, \tag{2}$$

where ψ_i and V_i are shorthand notations for $\psi(x_i)$ and $V(x_i)$, and $\Delta = x_{i+1} - x_i$ (the grid is equidistant). In a scattering problem i runs from $-\infty$ to ∞, leading to an infinite number of equations. This is awkward and unnecessary, since the scattering potential is localized in space, i.e. $V(x)$ differs from a constant only for $x_1 \leq x \leq x_N$. For the left and right regions, $x < x_1$ and $x > x_N$, the solutions to the Schrödinger equation are simple plane waves, see Fig. 3, with

$$k_L = \frac{\sqrt{2m(E-V_L)}}{\hbar}\ ;\ k_R = \frac{\sqrt{2m(E-V_R)}}{\hbar}. \tag{3}$$

To obtain a full solution of the Schrödinger equation, we only need to match these "modes" to the wave function in the region of the potential barrier (the scattering region).

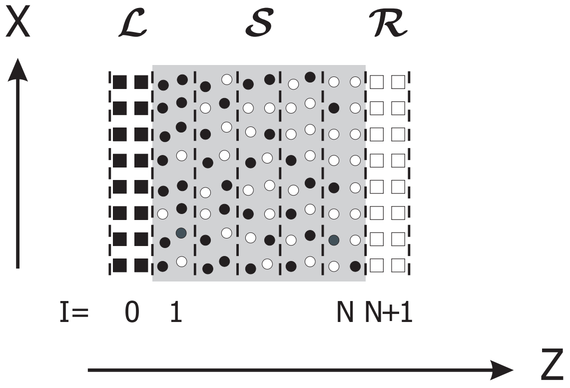

Figure 2: The semi-infinite leads and corresponding Hamiltonian problem with an infinite number of layers from Fig. 1 is replaced by finite leads and an effective Hamiltonian. The effective Hamiltonian is simply constructed by adding the energy-dependent self-energies $\Sigma_{\mathcal{L}}$ and $\Sigma_{\mathcal{R}}$ to the $\mathcal{H}_{0,0}$ and $\mathcal{H}_{N+1,N+1}$ Hamiltonian blocks, respectively, where the indices are principal layer indices. The lead atoms modified by the self energy are depicted as squares. The left and right self-energies are constructed in terms of generalized Bloch matrices and blocks of lead hopping matrices for the left-hand and right-hand leads, respectively.

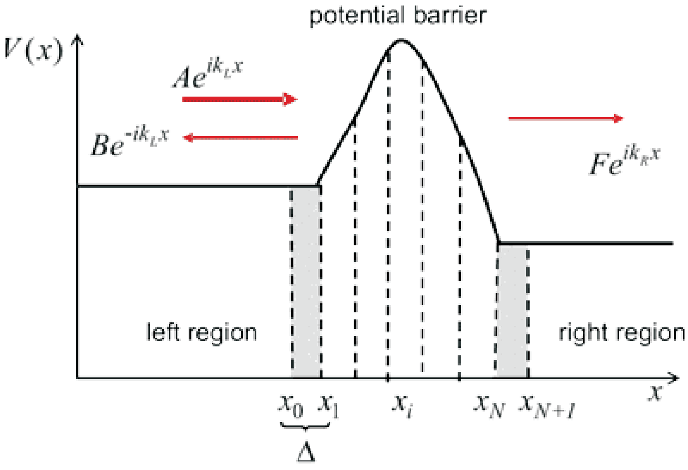

Figure 3: Discretization of a potential barrier. An equidistant grid is applied with $\Delta = x_{i+1} - x_i$. The potential is different from a constant for $x_1 \le x \le x_N$. The coupling to the left and right regions (the leads) can be included by extending the grid by two points, which defines the boundary zones, indicated in gray.

The finite difference Schrödinger equation for $i = 0$ is

$$E\psi_0 + \frac{\hbar^2}{2m\Delta^2}\left\{\psi_1 - 2\psi_0 + \psi_{-1}\right\} - V_0\psi_0 = 0. \tag{4}$$

We set $x_0 = 0$. For $x < 0$ the wave function has the form $\psi(x) = Ae^{ik_Lx} + Be^{-ik_Lx}$, so

$$\psi_{-1} = Ae^{-ik_L\Delta} + Be^{ik_L\Delta} = Ae^{-ik_L\Delta} + (\psi_0 - A)\, e^{ik_L\Delta}, \tag{5}$$

since the wave function is continuous at $x = 0$. In a scattering problem we assume that we have set the incoming wave, so A is fixed. Eq. 4 is rewritten as

$$E\psi_0 + \frac{\hbar^2}{2m\Delta^2}\left\{\psi_1 - 2\psi_0 + e^{ik_L\Delta}\psi_0\right\} - V_0\psi_0 = \frac{\hbar^2}{2m\Delta^2}A\left\{e^{ik_L\Delta} - e^{-ik_L\Delta}\right\}. \tag{6}$$

The term on the left-hand side only contains ψ_i with $i \geq 0$, and the terms on the right-hand side can be considered as a source term. This manipulation takes care of the left boundary.

For the right boundary we use a similar trick. For $i = N + 1$ we have

$$E\psi_{N+1} + \frac{\hbar^2}{2m\Delta^2}\left\{\psi_{N+2} - 2\psi_{N+1} + \psi_N\right\} - V_{N+1}\psi_{N+1} = 0. \tag{7}$$

Using

$$\psi_{N+2} = Fe^{ik_R(N+2)\Delta} = \psi_{N+1}e^{ik_R\Delta} \tag{8}$$

one obtains

$$E\psi_{N+1} + \frac{\hbar^2}{2m\Delta^2}\left\{\psi_{N+1}e^{ik_R\Delta} - 2\psi_{N+1} + \psi_N\right\} - V_{N+1}\psi_{N+1} = 0. \tag{9}$$

In Eq. 8 we have assumed only a transmitted wave on the right and no incoming wave. The term on the left-hand side of Eq. 9 contains only ψ_i with $i \leq N + 1$. This manipulation takes care of the right boundary.

For $i = 1, \ldots, N$ we use Eq. 2 in unaltered form. Collecting Eqs. 2, 6 and 9 the scattering problem can be written as

$$\left(E\mathbf{I} - \mathbf{H}'\right)\boldsymbol{\psi} = \mathbf{q}. \tag{10}$$

Here $\boldsymbol{\psi}$ is a vector containing the coefficients ψ_i; $i = 0, \ldots, N + 1$; $\mathbf{q}$ is the "source" vector of length $N + 2$. Only its first coefficient is nonzero

$$q_0 = \frac{\hbar^2}{2m\Delta^2}A\left\{e^{ik\Delta} - e^{-ik\Delta}\right\}. \tag{11}$$

$\mathbf{H}'$ is the $(N + 2) \times (N + 2)$ Hamiltonian matrix. It is tridiagonal with most of its elements identical to those of the original finite difference Hamiltonian

$$H'_{i,i+1} = H'_{i,i-1} = -\frac{\hbar^2}{2m\Delta^2}, \tag{12}$$

$$H'_{i,i} = -\frac{\hbar^2}{m\Delta^2} + V_i, \tag{13}$$

except for the first and the last diagonal elements, which are modified to

$$\begin{aligned} H'_{0,0} &= -\frac{\hbar^2}{m\Delta^2} + V_0 + \Sigma_L(E), \\ H'_{N+1,N+1} &= -\frac{\hbar^2}{m\Delta^2} + V_{N+1} + \Sigma_R(E), \end{aligned} \tag{14}$$

with

$$\begin{aligned} \Sigma_L(E) &= -\frac{\hbar^2}{2m\Delta^2}e^{ik_L\Delta}, \\ \Sigma_R(E) &= -\frac{\hbar^2}{2m\Delta^2}e^{ik_R\Delta}. \end{aligned} \tag{15}$$

In Green function jargon $\Sigma_{L/R}(E)$ are called the self-energies of the left and right leads. They take care of the coupling of the potential barrier to the outer regions, and contain all the required information about the outer regions. The self-energy depends upon the energy of the incoming and scattered waves through Eq. 3. Whereas Eq. 2 represents an infinite dimensional problem, we have reduced it to a finite, $N+2$ dimensional problem, Eq. 10. It can be solved using standard algorithms for solving linear equations, such as Gaussian elimination. In this case it is particularly simple, since the matrix is tridiagonal.

Once Eq. 10 is solved, it remains to extract the transmission and reflection amplitudes. The transmission amplitude is given by the wave function on the right side of the barrier, normalized to the amplitude of the incoming wave, and (flux) normalized with the velocities to obtain a unitary scattering matrix [43]

$$t = \sqrt{\frac{v_R}{v_L}} \frac{\psi_{N+1}}{A}. \tag{16}$$

The reflection amplitude is similarly determined from the wave function on the left side minus the incoming wave, normalized to the incoming wave

$$r = \frac{\psi_0 - A}{A}. \tag{17}$$

Some care should be taken in determining the velocities. Since we have discretized the Schrödinger equation, it is consistent to discretize the expression for the current in a similar way

$$J = \frac{i\hbar}{2m}\left(\psi_i \frac{\psi_{i+1}^* - \psi_i^*}{\Delta} - \psi_i^* \frac{\psi_{i+1} - \psi_i}{\Delta}\right). \tag{18}$$

For a simple plane wave Ae^{ikx} this expression gives

$$J = \frac{i\hbar\,|A|^2}{2m\Delta}\left(e^{-ik\Delta} - e^{ik\Delta}\right),$$

Since J is particle density $|A|^2$ times velocity v, one obtains

$$v = \frac{i\hbar}{2m\Delta}\left(e^{-ik\Delta} - e^{ik\Delta}\right). \tag{19}$$

The source term, Eq. 11, can then be simplified to

$$q_0 = \frac{i\hbar A}{\Delta} v_L. \tag{20}$$

From Eqs. 19 and 15 one can relate the velocity to the self-energy

$$v_{L/R} = -\frac{2\Delta}{\hbar}\,\mathrm{Im}\,\Sigma_{L/R}(E). \tag{21}$$

Green function expressions

Using Green functions these results can be put into a very compact, albeit somewhat obscure, form. One can define a Green function matrix by

$$\mathbf{G}(E) = (E\mathbf{I} - \mathbf{H}')^{-1}. \tag{22}$$

It has dimensions $N+2$, like the modified Hamiltonian matrix $\mathbf{H}'$. One can also define the infinite dimensional retarded Green function matrix related to the original infinite dimensional Hamiltonian

$$\mathbf{G}^r(E) = [(E + i\eta)\mathbf{I} - \mathbf{H}]^{-1}, \tag{23}$$

where η is (real, positive) infinitesimal. For z a complex number in the lower half plane, the matrix elements of $\mathbf{G}(z)$ and $\mathbf{G}^r(z)$ in the scattering region are identical [43]. Note that $\mathbf{H}'$ is non-Hermitian, because the self-energy Σ is complex, see Eqs. 14 and 15. One can show that the eigenvalues of $\mathbf{H}'$ are

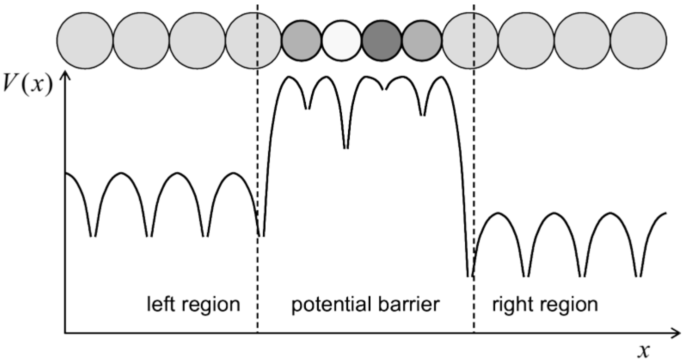

Figure 4: *Top*: atomic chain. The leads (left and right region) are periodic chains of identical atoms. The middle region contains different atoms and/or disorder. *Bottom*: schematic representation of the potential along the chain.

not real and lie in the upper half complex plane. Thus $\mathbf{G}(E)$ is a well-defined quantity for real energies E. By construction it has the retarded boundary condition build into it and one does not need the usual $+i\eta$ trick.

The definition of $\mathbf{G}$ allows us to write

$$\psi_{N+1} = G_{N+1,0}(E)q_0, \tag{24}$$

see Eq. 10. Eqs. 16, 20 and 24 then lead to a compact Fisher-Lee expression for the transmission amplitude [24]

$$t = \frac{i\hbar}{\Delta}\sqrt{v_R v_L}\, G_{N+1,0}(E), \tag{25}$$

which relates matrix elements of the scattering matrix to matrix elements of the Green function. Using Eq. 21 we can write

$$t = 2i\sqrt{-\operatorname{Im}\Sigma_R}\, G_{N+1,0}(E)\, \sqrt{-\operatorname{Im}\Sigma_L}, \tag{26}$$

which allows the transmission coefficient to be written as

$$T = t^* t = 4(\operatorname{Im}\Sigma_R)G^r_{N+1,0}(\operatorname{Im}\Sigma_L)G^a_{0,N+1}, \tag{27}$$

with all quantities evaluated at a fixed energy E, and $\mathbf{G}^a = [\mathbf{G}^r]^\dagger$ the advanced Green-function matrix. Eq. 27 is known as the Caroli expression [23]. Its generalization to finite bias, i.e. to the non-linear response regime, is also known as the non-equilibrium Green function or NEGF expression.

1.1.2 Tight binding

Wave function matching can be extended straightforwardly to LCAO (linear combinations of atomic orbitals) and tight-binding (TB: nearest-neighbour interactions only) Hamiltonians. We illustrate this in one dimension for the atomic wire sketched in Fig. 4.

In the LCAO approximation, wave functions are expanded in a basis set of fixed atomic orbitals $\psi(x) = \sum_i c_i \chi_i(x - X_i)$,where X_i denote the positions of the atoms. The wave function is then represented by the column vector of the coefficients

$$\boldsymbol{\psi} = \begin{pmatrix} \vdots \\ c_{i-1} \\ c_i \\ c_{i+1} \\ \vdots \end{pmatrix}. \tag{28}$$

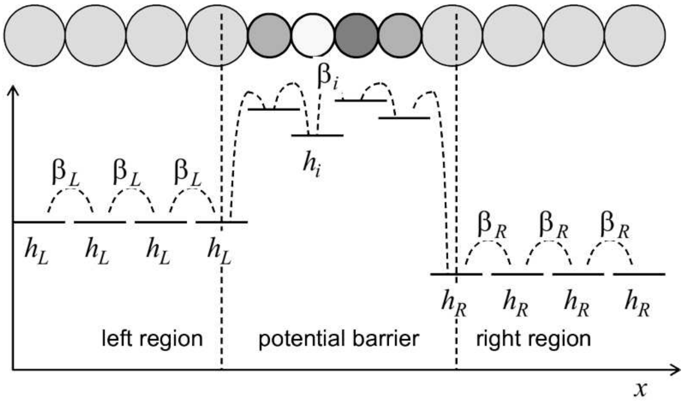

Figure 5: Nearest neighbor tight-binding model of an atomic chain. The periodic left and right regions are characterized by the on-site and hopping matrix elements $h_{L/R}$ and $\beta_{L/R}$. The scattering region has site dependent matrix elements h_i and β_i.

Since we solve a scattering problem, the atomic orbitals cover all space, and the vector has infinite dimension, i.e. $i = -\infty, \ldots, \infty$. The Schrödinger equation becomes

$$(E\mathbf{I} - \mathbf{H})\,\boldsymbol{\psi} = \mathbf{0}, \tag{29}$$

with $\mathbf{H}$ the Hamiltonian matrix with matrix elements $H_{i,j} = \langle \chi_i | \widehat{H} | \chi_j \rangle$. To keep things simple we assume that the atomic orbital basis is orthonormal.[2] We use a single atomic orbital per site and we assume nearest neighbor interactions only (tight-binding). The diagonal elements of $\mathbf{H}$ are $H_{i,i} = h_i$; its off-diagonal elements are $H_{i+1,i} = \beta_i$, $H_{i,i+1} = \beta_i^*$ and all elements $H_{j,i} = 0$ for $j > i+1$ and $j < i-1$. The (Hermitian) Hamiltonian matrix is then

$$\mathbf{H} = \begin{pmatrix} \ddots & \cdots & 0 & 0 & \\ \vdots & h_{i-1} & \beta_{i-1}^* & 0 & 0 \\ 0 & \beta_{i-1} & h_i & \beta_i^* & 0 \\ 0 & 0 & \beta_i & h_{i+1} & \vdots \\ & 0 & 0 & \cdots & \ddots \end{pmatrix}. \tag{30}$$

None of these approximations is essential and the WFM formalism can be made to work for any LCAO representation; here we just want to keep the notation as simple as possible.

As before, we divide our system into three parts: a left lead, a scattering region, and a right lead. The left and right leads are crystalline materials with translational symmetry. Matrix elements in the leads must be site-independent, i.e. $h_i = h_{L/R}$ and $\beta_i = \beta_{L/R}$ for the left/right leads. Only in the scattering region do we have site-dependent matrix elements. The basic idea is illustrated in Fig. 5.

Ideal lead modes

Writing out Eq. 29 in its components gives

$$-\beta_{i-1} c_{i-1} + (E - h_i) c_i - \beta_i^* c_{i+1} = 0, \tag{31}$$

with i running from $-\infty$ to ∞. These equations have the same form as the discretized Schrödinger equation of Eq. 2 if we make the substitutions

$$c_i \to \psi_i \quad ; \quad h_i \to -\frac{\hbar^2}{m\Delta^2} + V_i \quad ; \quad \beta_i \to -\frac{\hbar^2}{2m\Delta^2}.$$

---

[2] For non-orthogonal basis sets one introduces an overlap matrix $\mathbf{S}$, with matrix elements $S_{i,j} = \langle \chi_i | \chi_j \rangle$, and replaces $\mathbf{I}$ by $\mathbf{S}$.

As before, the scattering problem is solved by WFM. First we have to find the modes of the ideal leads. For sites i in the left lead the matrix elements are site independent and Eq. 31 becomes

$$-\beta_L c_{i-1} + (E - h_L)c_i - \beta_L^* c_{i+1} = 0. \tag{32}$$

This equation has the same form as a discretized Schrödinger equation for a particle in a constant potential, so the solutions are discretized plane waves, i.e.

$$c_n = Ae^{ik_L n a_L}, \tag{33}$$

where the distance between the atoms a_L is the "discretization step". The same holds for the right lead, replacing the subscript L by R.

One could derive this in a somewhat more formal way. As a consequence of the Bloch-Floquet theorem the functions in consecutive cells of a periodic system are related by a constant amplitude/phase factor λ, i.e.

$$\text{if } \ c_{i-1} = c \ \text{ then } \ c_i = \lambda c \ \text{ and } \ c_{i+1} = \lambda^2 c. \tag{34}$$

Assuming for simplicity that β is real, Eq. 32 gives

$$\begin{aligned} -\beta + (E-h)\lambda - \beta\lambda^2 = 0 \Rightarrow \\ \lambda = \frac{E-h}{2\beta} \pm \left[\left(\frac{E-h}{2\beta}\right)^2 - 1\right]^{\frac{1}{2}}, \end{aligned} \tag{35}$$

where you add the subscript L/R for the left and right leads. The roots λ can be given a more familiar form. For $\left|\frac{E-h}{2\beta}\right| \leq 1$ we define a wave number k by[3]

$$\cos(ka) = \frac{E-h}{2\beta}, \tag{36}$$

which leads to the simple form

$$\lambda_\pm = e^{\pm ika}, \tag{37}$$

i.e. the familiar form of the Bloch factor. Using Eq. 34 recursively, i.e. $c_n = \lambda^n c_0$, then leads to Eq. 33, with $A = c_0$. It describes propagating waves, with λ_+ a wave propagating to the right, and λ_- a wave propagating to the left.

For $\left|\frac{E-h}{2\beta}\right| > 1$ one can define κ by

$$\cosh(\kappa a) = \left|\frac{E-h}{2\beta}\right|, \tag{38}$$

and obtain

$$\begin{aligned} \lambda_\pm &= +e^{\mp\kappa a} \ \text{ if } \ \frac{E-h}{2\beta} > 1; \\ \lambda_\pm &= -e^{\mp\kappa a} \ \text{ if } \ \frac{E-h}{2\beta} < -1. \end{aligned} \tag{39}$$

Both these cases describe waves that decay either to the right or to the left, i.e. evanescent waves. They are not acceptable as solutions to the one-dimensional Schrödinger equation since one cannot normalize them. However, we have a use for them in three-dimensional problems, as we will see later on.

Wave function matching

Having obtained the modes of the ideal leads, we match them to the scattering region, where the matrix elements h_i and β_i in Eq. 31 are site dependent. We assume that the scattering region is localized in

---

[3] $E(k) = h + 2\beta\cos ka$ is of course the dispersion relation of a 1D s-band in the nearest neighbour tight-binding model.

space, so i runs from 1 to N. The procedure we have used to solve the discretized Schrödinger problem in Sec. 1.1.1 can be copied with only small modifications. Using Eq. 37, Eqs. 5 and 8 read[4]

$$\begin{aligned} c_{-1} &= A\lambda_{L,+}^{-1} + B\lambda_{L,-}^{-1} = A\lambda_{L,+}^{-1} + (c_0 - A)\,\lambda_{L,-}^{-1}; \\ c_{N+2} &= c_{N+1}\lambda_{R,+}. \end{aligned} \tag{40}$$

Eq. 40 can be used to substitute Eq. 29 by

$$(E\mathbf{I} - \mathbf{H}')\,\boldsymbol{\psi} = \mathbf{q}, \tag{41}$$

similar to Eq. 10. $\boldsymbol{\psi}$ is a finite dimensional vector that contains the coefficients c_i in the scattering region plus those in the two boundaries, i.e. $i = 0, \ldots, N+1$. $\mathbf{q}$ is the "source" vector of length $N+2$, whose coefficients are zero, except the first one

$$q_0 = \beta_L A \left\{ \lambda_{L,-}^{-1} - \lambda_{L,+}^{-1} \right\}. \tag{42}$$

$\mathbf{H}'$ is a finite $(N+2) \times (N+2)$ Hamiltonian matrix. All its matrix elements are identical to that of the original Hamiltonian matrix, Eq. 30, except for the first and the last diagonal element, which are modified to

$$\begin{aligned} H'_{0,0} &= h_0 + \Sigma_L(E); \\ H'_{N+1,N+1} &= h_{N+1} + \Sigma_R(E), \end{aligned} \tag{43}$$

with

$$\begin{aligned} \Sigma_L(E) &= \beta_L \lambda_{L,-}^{-1}; \\ \Sigma_R(E) &= \beta_R \lambda_{R,+}. \end{aligned} \tag{44}$$

These "self-energies" contain all the information concerning the coupling of the scattering region to the leads. As before, they are complex and energy dependent through Eqs. 36 and 37.

We have replaced an infinite dimensional problem, Eq. 29, by a finite dimensional one, Eq. 41. The latter has the same form as Eq. 10. Since "the same equations have the same solutions", the transmission amplitude of Eq. 16 becomes

$$t = \sqrt{\frac{v_R}{v_L}} \frac{c_{N+1}}{A} \tag{45}$$

with, as in Eq. 21, the velocities given by

$$v_{L/R} = -\frac{2a_{L/R}}{\hbar} \operatorname{Im} \Sigma_{L/R}(E). \tag{46}$$

Using WFM, simple scattering problems with tight-binding Hamiltonians can be solved analytically in a straightforward way, as illustrated in Refs. [27,32] The Green function expressions given in Sec. 1.1.1 are also valid for tight-binding Hamiltonians.

1.1.3 Wave function matching in three dimensions

In this section we generalize WFM to problems in three dimensions. We use Landauer's formula to express the conductance in terms of the transmission amplitudes $t_{n,m}$, see Eq. 1. We will see that calculating transmission amplitudes for scattering in layered systems in three dimensions is conceptually similar to the one-dimensional case.

---

[4] We write $c_{i+n} = \lambda_{\pm}^{n} c_i$, where n is an integer (positive or negative), and let the ± indicate waves propagating to the left and right, respectively. In the one-dimensional case, one always has $\lambda_+ = 1/\lambda_-$. In the three-dimensional case, this relation does not necessarily hold. We use a notation that is easily generalized to three dimensions.

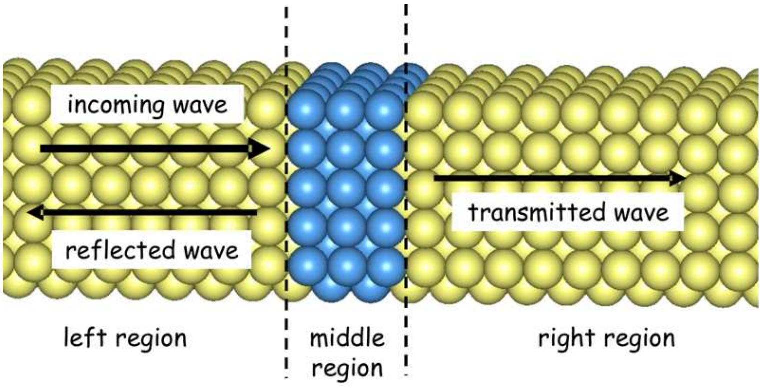

Figure 6: Schematic representation of a tunnel junction. The yellow balls represent atoms of a metal, the blue balls represent atoms of an insulator. The left and right regions stretch macroscopically far into the left and right, respectively. The electron waves in the metal are reflected or transmitted by the insulator in the middle region

As an example we consider the tunnel junction shown in Fig. 6. The principal idea is to divide the system into layers of atoms, normal to the transport direction. One chooses the layers sufficiently thick that the Hamiltonian matrix only contains matrix elements that either couple atoms within one layer, or atoms that are in nearest neighbor layers.[5] The Hamiltonian matrix of Eq. 30 becomes

$$\mathbf{H} = \begin{pmatrix} \ddots & \cdots & 0 & 0 & \\ \vdots & \mathbf{H}_{i-1} & \mathbf{B}^{\dagger}_{i-1} & 0 & 0 \\ 0 & \mathbf{B}_{i-1} & \mathbf{H}_i & \mathbf{B}^{\dagger}_i & 0 \\ 0 & 0 & \mathbf{B}_i & \mathbf{H}_{i+1} & \vdots \\ & 0 & 0 & \cdots & \ddots \end{pmatrix}, \tag{47}$$

with $i = -\infty, \ldots, \infty$. The matrices $\mathbf{H}_i$ contain the interactions between atoms within layer i, and $\mathbf{B}_i$ describe the coupling between layers i and $i+1$. Both are $N \times N$ matrices, with N the total number of atomic orbitals of all atoms in a layer. The scattering region is localized in the layers $i = 1, \ldots, S$. A schematic representation of the structure of the Hamiltonian is given Fig. 7.[6]

This representation is valid both for systems with a finite cross section (i.e. wires), and for infinite layered systems that are periodic along the interfaces. In the latter case N refers to the number of atoms within the unit cell. $\mathbf{k}_{\|}$ is then a good quantum number and the matrices $\mathbf{H}_i(\mathbf{k}_{\|})$ depend on this quantum number. The exact forms of these matrices are not important here and to simplify the notation we will omit the quantum number $\mathbf{k}_{\|}$. Moreover, we will use the phrase "wire" to indicate both systems with a finite cross section and systems with infinite periodic interfaces.

---

[5] The formalism can be extended straightforwardly to include interactions of a longer range, but the notation becomes a bit messy, so we consider only nearest neighbour interactions here.

[6] Note that the notation has changed slightly here. Now N is the dimension of the basis *within* one layer, and S is the *number* of layers in the scattering region. Sorry about that.

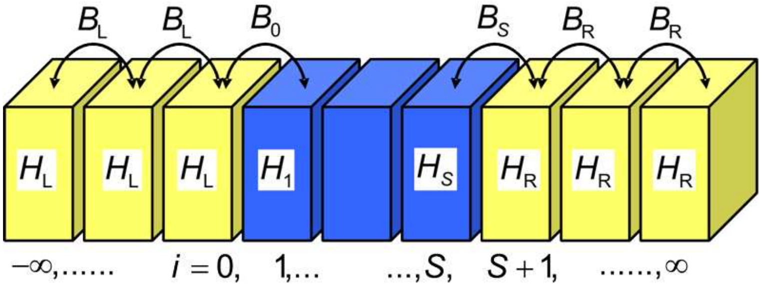

Figure 7: Hamiltonian of a tunnel junction divided into layers. The transport direction is along the horizontal. The left (L) and right (R) leads are ideal periodic wires containing the layers $i = -\infty, \ldots, 0$ and $i = S{+}1, \ldots, \infty$, respectively. The layers $i = 1, \ldots, S$ consitute the scattering region.

The wave function of Eq. 28 is generalized to

$$\boldsymbol{\psi} = \begin{pmatrix} \vdots \\ \mathbf{c}_{i-1} \\ \mathbf{c}_i \\ \mathbf{c}_{i+1} \\ \vdots \end{pmatrix}, \tag{48}$$

where $\mathbf{c}_i$ is a vector of dimension N. As in Sec. 1.1.2 we divide our system into three parts, with $i = -\infty, \ldots, 0$ corresponding to the left lead (L), $i = 1, \ldots, S$ to the scattering region (S) and $i = S{+}1, \ldots, \infty$ to the right lead (R). Within WFM the scattering problem is again solved in two steps. First the Bloch modes of the leads are calculated, then these are matched to the scattering region.

Ideal lead modes

The leads are assumed to be ideal wires characterized by a periodic potential. The "principal" layer is a multiple of the translational period along the wire. By construction, the Hamiltonian matrix for each layer is identical, i.e. $\mathbf{H}_i = \mathbf{H}_{L/R}$ and $\mathbf{B}_i = \mathbf{B}_{L/R}$ for the left/right leads, see Fig. 7. Eq. 32 is generalized to

$$-\mathbf{B}_{L/R}\mathbf{c}_{i-1} + (E\mathbf{1} - \mathbf{H}_{L/R})\mathbf{c}_i - \mathbf{B}^{\dagger}_{L/R}\mathbf{c}_{i+1} = 0, \tag{49}$$

with $\mathbf{1}$ the $N \times N$ identity matrix.[7] We make the same ansatz as in Eq. 34, namely that the coefficients in successive layers are connected by a Bloch factor λ

$$\mathbf{c}_{i-1} \equiv \mathbf{c} \quad ; \quad \mathbf{c}_i = \lambda\mathbf{c} \quad ; \quad \mathbf{c}_{i+1} = \lambda\mathbf{c}_i = \lambda^2\mathbf{c} \tag{50}$$

and get the equation

$$-\mathbf{B}\mathbf{c} + \lambda(E\mathbf{1} - \mathbf{H})\mathbf{c} - \lambda^2\mathbf{B}^{\dagger}\mathbf{c} = 0, \tag{51}$$

where the subscripts L/R have been omitted to simplify the notation. We work at a fixed energy E, and Eq. 51 is a quadratic eigenvalue equation dimension N. The standard trick to solve such an equation is to define $\mathbf{d} = \lambda\mathbf{c}$ and convert it into

$$\left[\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{B} & E\mathbf{1} - \mathbf{H} \end{pmatrix} - \lambda \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}^{\dagger} \end{pmatrix}\right]\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} = 0. \tag{52}$$

This is a generalized linear eigenvalue problem of dimension $2N$, which can be solved using standard numerical techniques.

---

[7] For non-orthogonal basis sets one replaces $\mathbf{1}$ by $\mathbf{S}$, the overlap matrix.

It can be shown that this equation generally has $2N$ solutions, which can be divided into N right-going modes and N left-going modes, labeled by "+" and "−" subscripts as in Eqs. 37 and 39. Right-going modes are either evanescent waves that are decaying to the right, or waves of constant amplitude that are propagating to the right, whereas left-going modes are decaying or propagating to the left. In contrast to the one-dimensional case, we find in three dimensions at a fixed energy in general both evanescent and propagating modes. We denote the eigenvalues and eigenvectors of Eq. 51 by

$$\lambda_{\pm,n} \quad ; \quad \mathbf{u}_{\pm,n} \quad ; \quad n = 1, \ldots, N. \tag{53}$$

Together these states form a complete basis set. In the following we assume that the vectors $\mathbf{u}_{\pm,n}$ are normalized. Note however that in general they are not orthogonal. One can easily distinguish right- from left-going evanescent modes on the basis of their eigenvalues. Right-going evanescent modes have $|\lambda_{+,n}| < 1$ and left-going evanescent modes have $|\lambda_{-,n}| > 1$, see Eq. 50. Propagating modes per definition have $|\lambda_{\pm,n}| = 1$, so here one has to determine the Bloch velocity in the propagation direction and use its sign to distinguish right from left propagation. One can show that for a tight-binding Hamiltonian, the general expression for the Bloch velocities becomes

$$v_{\pm,n} = -\frac{2a}{\hbar} \operatorname{Im}\left[\lambda_{\pm,n}\mathbf{u}^{\dagger}_{\pm,n}\mathbf{B}^{\dagger}\mathbf{u}_{\pm,n}\right], \tag{54}$$

where a is the thickness of the layer [27]. In addition one can show that the Bloch velocity is non-zero only for propagating modes, i.e. evanescent states have a Bloch velocity equal to zero, as one expects on physical grounds.

Since the eigenvectors are non-orthogonal, it is convenient to define dual vectors $\widetilde{\mathbf{u}}_{\pm,n}$ by

$$\widetilde{\mathbf{u}}^{\dagger}_{\pm,n}\mathbf{u}_{\pm,m} = \delta_{n,m} \quad ; \quad \mathbf{u}^{\dagger}_{\pm,n}\widetilde{\mathbf{u}}_{\pm,m} = \delta_{n,m}. \tag{55}$$

Any wave function in the leads can be expressed as a linear combination of the lead modes. This can be done in a very compact way if we define the two $N \times N$ Bloch matrices for right- and left-going modes

$$\mathbf{F}_{\pm} = \sum_{n=1}^{N} \lambda_{\pm,n}\mathbf{u}_{\pm,n}\widetilde{\mathbf{u}}^{\dagger}_{\pm,n}. \tag{56}$$

These generalize the Bloch factors of the one-dimensional case, see Eqs. 37 and 39. One can easily construct powers of Bloch matrices

$$\mathbf{F}^{i}_{\pm} = \sum_{n=1}^{N} \lambda^{i}_{\pm,n}\mathbf{u}_{\pm,n}\widetilde{\mathbf{u}}^{\dagger}_{\pm,n}. \tag{57}$$

This expression is valid for any integer i, positive or negative. A general solution in the leads can now be expressed by a recursion relation

$$\mathbf{c}_i = \mathbf{c}_{+,i} + \mathbf{c}_{-,i} = \mathbf{F}^{i-j}_{+}\mathbf{c}_{+,j} + \mathbf{F}^{i-j}_{-}\mathbf{c}_{-,j}. \tag{58}$$

In a scattering problem one usually fixes the coefficients in one layer by suitable boundary conditions. Using Eq. 58 one can then determine the solution in all the layers of the leads.

Wave function matching

The recursion relations are used to set up equations that properly match the leads to the scattering region. The scattering region is defined by the layers $i = 1, \ldots, S$, see Fig. 7. Immediately left of the scattering regions one has the recursion relation

$$\mathbf{c}_{-1} = \mathbf{F}^{-1}_{L,+}\mathbf{c}_{+,0} + \mathbf{F}^{-1}_{L,-}\mathbf{c}_{-,0}.$$

Writing $\mathbf{c}_{-,0} = \mathbf{c}_0 - \mathbf{c}_{+,0}$ one gets

$$\mathbf{c}_{-1} = \left[\mathbf{F}^{-1}_{L,+} - \mathbf{F}^{-1}_{L,-}\right]\mathbf{c}_{+,0} + \mathbf{F}^{-1}_{L,-}\mathbf{c}_0. \tag{59}$$

We introduce the scattering boundary condition as follows. The vector $\mathbf{c}_{+,0}$ is treated as the source, i.e. as the incoming wave from the left lead, e.g. a specific propagating mode of the left lead.

$$\mathbf{c}_{+,0} = \mathbf{u}_{L,+,m}. \tag{60}$$

Immediately to the right of the scattering region one has

$$\mathbf{c}_{S+2} = \mathbf{F}_{R,+}\mathbf{c}_{+,S+1} + \mathbf{F}_{R,-}\mathbf{c}_{-,S+1}.$$

We have no incoming wave from the right lead, i.e. $\mathbf{c}_{-,S+1} = 0$, so

$$\mathbf{c}_{S+2} = \mathbf{F}_{R,+}\mathbf{c}_{S+1}. \tag{61}$$

Eqs. 59 and 61 can now be used to “simplify” the tight-binding equations

$$-\mathbf{B}_i\mathbf{c}_{i-1} + (E\mathbf{1} - \mathbf{H}_i)\mathbf{c}_i - \mathbf{B}_i^\dagger\mathbf{c}_{i+1} = 0. \tag{62}$$

For $i = 0$ we write

$$\begin{aligned}
&-\mathbf{B}_L\mathbf{c}_{-1} + (E\mathbf{1} - \mathbf{H}_L)\mathbf{c}_0 - \mathbf{B}_1^\dagger\mathbf{c}_1 = 0 \Leftrightarrow \\
&(E\mathbf{1} - \mathbf{H}_L - \mathbf{B}_L\mathbf{F}_{L,-}^{-1})\mathbf{c}_0 - \mathbf{B}_1^\dagger\mathbf{c}_1 = \mathbf{B}_L\left[\mathbf{F}_{L,+}^{-1} - \mathbf{F}_{L,-}^{-1}\right]\mathbf{u}_{L,+,m}.
\end{aligned} \tag{63}$$

Likewise for $i = S+1$ we write

$$\begin{aligned}
&-\mathbf{B}_S\mathbf{c}_S + (E\mathbf{1} - \mathbf{H}_R)\mathbf{c}_{S+1} - \mathbf{B}_R^\dagger\mathbf{c}_{S+2} = 0 \Leftrightarrow \\
&-\mathbf{B}_S\mathbf{c}_S + (E\mathbf{1} - \mathbf{H}_R - \mathbf{B}_R^\dagger\mathbf{F}_{R,+})\mathbf{c}_{S+1} = 0.
\end{aligned} \tag{64}$$

Eq. 62 with $i = 1, \ldots, S$, and Eqs. 63 and 64 are collected

$$(E\mathbf{1} - \mathbf{H}')\psi = \mathbf{Q}_{L,+,m}, \tag{65}$$

with

$$\mathbf{H}' = \begin{pmatrix}
\mathbf{H}_L + \boldsymbol{\Sigma}_L(E) & \mathbf{B}_1^\dagger & 0 & 0 & 0 \\
\mathbf{B}_1 & \ddots & \mathbf{B}_{i-1}^\dagger & 0 & 0 \\
0 & \mathbf{B}_{i-1} & \mathbf{H}_i & \mathbf{B}_i^\dagger & 0 \\
0 & 0 & \mathbf{B}_i & \ddots & \mathbf{B}_S^\dagger \\
0 & 0 & 0 & \mathbf{B}_S & \mathbf{H}_R + \boldsymbol{\Sigma}_R(E)
\end{pmatrix}, \tag{66}$$

and

$$\boldsymbol{\psi} = \begin{pmatrix} \mathbf{c}_0 \\ \vdots \\ \mathbf{c}_i \\ \vdots \\ \mathbf{c}_{S+1} \end{pmatrix} \quad ; \quad \mathbf{Q}_{L,+,m} = \begin{pmatrix} \mathbf{B}_L\left[\mathbf{F}_{L,+}^{-1} - \mathbf{F}_{L,-}^{-1}\right]\mathbf{u}_{L,+,m} \\ \vdots \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}. \tag{67}$$

As in Eq. 44 the quantities

$$\begin{aligned}
\boldsymbol{\Sigma}_L(E) &= \mathbf{B}_L\mathbf{F}_{L,-}^{-1}; \\
\boldsymbol{\Sigma}_R(E) &= \mathbf{B}_R^\dagger\mathbf{F}_{R,+},
\end{aligned} \tag{68}$$

are called the “self-energies” of the left and right leads. They contain all the information about the coupling of the scattering region to the leads, as well as information on the scattering boundary conditions. The self-energies depend upon the energy E, since they are expressed in the Bloch matrices and thus in the lead modes and the latter have been determined at a fixed energy E. The self-energies are non-Hermitian, which makes the Hamiltonian $\mathbf{H}'$ non-Hermitian. Eq. 65 represents a set of linear equations of dimension $(S+2)\times N$. These can be solved using common techniques, e.g. Gaussian elimination (LU decomposition), followed by back substitution. Since the matrix $\mathbf{H}'$ has a block tridiagonal form (with blocks of dimension N), one can make use of this form to optimize the Gaussian elimination algorithm. Alternatively, since the matrices are quite sparse, one can make use of special sparse matrix techniques to solve this problem.

Transmission matrix elements are obtained by expanding the wave function in the right lead into modes

$$\mathbf{c}_{S+1} = \sum_{n-1}^{N} \mathbf{u}_{R,+,n} t'_{n,m} \;\Rightarrow\; t'_{n,m} = \widetilde{\mathbf{u}}^{\dagger}_{R,+,n}\mathbf{c}_{S+1} \tag{69}$$

and (flux) normalize them with the velocities to ensure a unitary scattering matrix,

$$t_{n,m} = \sqrt{\frac{v_{L,+,m}}{v_{R,+,n}}\frac{a_R}{a_L}}\widetilde{\mathbf{u}}^{\dagger}_{R,+,n}\mathbf{c}_{S+1} \tag{70}$$

The velocities are calculated from Eq. 54. By letting m in Eqs. 60 and 67 run over all (propagating) modes $\mathbf{u}_{L,+,m}$ of the left lead, all transmission matrix elements are obtained. This sounds more complicated than it is. If one uses Gaussian elimination (LU decomposition) to solve Eq. 65 the elimination (decomposition) step is independent of the source vector $\mathbf{Q}_{L,+,m}$. This is the most time consuming algorithmic step. The source vector only enters in the second algorithmic step, i.e. back substitution, which is much cheaper and can easily be performed in parallel for the whole set of $\mathbf{Q}_{L,+,m}$. Moreover, if one is only interested in the transmission amplitudes, the back substitution step does not have to be fully completed, since one only needs the coefficients $\mathbf{c}_{S+1}$. If one uses sparse matrix techniques, it is possible to solve the set of linear equations in parallel for all source vectors.

Although WFM permits the calculation of amplitudes $t'_{n,m}$ of Eq. 69 between all states n and m, i.e. propagating and evanescent, only propagating states actually contribute to the transmission. Therefore, it is possible to restrict n and m to propagating states only. This does not mean that one can throw out the evanescent states altogether. One needs to include them in properly matching the scattering region to the leads, cf. Eq. 68. In other words, the Bloch matrices, Eq. 57, need to be constructed from all N modes, propagating and evanescent. Both of them are needed for a complete basis.

Green function expressions

WFM can be translated into Green function expressions at the cost of loosing some of its transparency [27]. With respect to the Hamiltonian matrix of Eq. 66 a finite Green function matrix can be defined as

$$\mathbf{G}(E) = (E\mathbf{1}-\mathbf{H}')^{-1}. \tag{71}$$

It can be calculated by matrix inversion using essentially the same block Gaussian elimination scheme as used for solving the set of linear equations, Eq. 65. The matrix $\mathbf{H}'$ is non-Hermitian; its eigenvalues are not real, so the Green function matrix can be evaluated for real energies.[8]

With respect to the original infinite Hamiltonian $\mathbf{H}$ of Eq. 47 one can define the usual retarded (infinite) Green function matrix

$$\mathbf{G}^r(E) = \left[(E+i\eta)\mathbf{1}-\mathbf{H}\right]^{-1}, \tag{72}$$

where one needs the infinitesimal η to avoid the poles on the real axis. One can show that for layers in the scattering region and $\lim_{\eta\rightarrow 0}$ one has

$$\mathbf{G}_{i,j}(E) = \mathbf{G}^r_{i,j}(E) \;\;;\;\; i,j=0,\ldots,S+1. \tag{73}$$

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[8] The exceptions are truly bound states of $\mathbf{H}'$. These occur at real energies, at which the Green function matrix has poles. However, these usually occur outside the energy range that is of interest for scattering. At bound state energies only evanescent modes exist in the leads, so this situation is easily identified in practice.

In terms of the Green function, the wave function in the scattering region can be written as

$$\psi = \mathbf{G}(E)\ \mathbf{Q}_{L,+,m}, \tag{74}$$

and from Eq. 69 one obtains

$$t_{n,m} = \sqrt{\frac{v_{L,+,m}}{v_{R,+,n}}\frac{a_R}{a_L}}\ \widetilde{\mathbf{u}}^{\dagger}_{R,+,n}\ \mathbf{G}_{S+1,0}(E)\ \mathbf{Q}_{L,+,m}. \tag{75}$$

After some manipulation one can obtain a Fisher-Lee expression that generalizes the one-dimensional expression of Eq. 25

$$t_{n,m} = i\hbar\sqrt{\frac{v_{R,+,n}v_{L,+,m}}{a_La_R}}\ \widetilde{\mathbf{u}}^{\dagger}_{R,+,n}\ \mathbf{G}_{S+1,0}(E)\ \widetilde{\mathbf{u}}'_{L,+,m}. \tag{76}$$

The notation becomes a bit messy because the modes $\mathbf{u}_{L/R,+,m/n}$ are not orthogonal. If they were orthogonal, then the expression would contain $\mathbf{u}^{\dagger}_{R,+,n}\mathbf{G}_{S+1,0}(E)\mathbf{u}_{L,+,m}$. The transmission amplitude from mode $\mathbf{u}_{L,+,m}$ in the left lead to mode $\mathbf{u}_{R,+,n}$ in the right lead is determined by the Green function matrix that takes you from layer $i = 0$ to layer $i = S + 1$, i.e. across the scattering region. Proper orthogonalization of the modes leads to expressions for $\widetilde{\mathbf{u}}^{\dagger}_{R,+,n}$ and $\widetilde{\mathbf{u}}'_{L,+,m}$. The expressions can be found in Ref. [27]. The Bloch velocities $v_{L/R,+,m/n}$ make the scattering matrix unitary. Since $v_{L/R,+,m/n} \neq 0$ only for propagating states, Eq. 76 expresses explicitly that the transmission is zero whenever n or m describes an evanescent mode. The layer thicknesses $a_{L/R}$ are normalization factors, since our modes are normalized within a layer.

Most of the Green function expressions we obtained in the one-dimensional case can be generalized to three dimensions. The velocity of Eq. 21 becomes a velocity matrix

$$\mathbf{V}_{L/R} = -\frac{2a_{L/R}}{\hbar}\,\mathrm{Im}\,\mathbf{\Sigma}_{L/R}. \tag{77}$$

The matrix is diagonal and has dimension N (the total number of modes). The diagonal matrix elements are the mode velocities $v_{L/R,\pm,n}$ of Eq. 54. Since $v_{L/R,\pm,n} = 0$ for evanescent states, the velocity matrices are in general singular. The transmission amplitudes of Eq. 76 can be collected in a transmission matrix $\mathbf{t}$

$$\mathbf{t} = 2i\sqrt{-\,\mathrm{Im}\,\mathbf{\Sigma}_R}\ \mathbf{G}_{S+1,0}(E)\ \sqrt{-\,\mathrm{Im}\,\mathbf{\Sigma}_L}, \tag{78}$$

which generalizes Eq. 26. The total transmission can be expressed as

$$T = \mathrm{Tr}\left[\mathbf{t}^{\dagger}\mathbf{t}\right] = 4\mathrm{Tr}\left[\mathrm{Im}\,\mathbf{\Sigma}_R\ \mathbf{G}^r_{S+1,0}(E)\ \mathrm{Im}\,\mathbf{\Sigma}_L\ \mathbf{G}^a_{0,S+1}(E)\right] \tag{79}$$

which generalizes Eq. 27 and is known as the Caroli expression or the NEGF expression [23].

2 Real space grid implementation: conductance of atomic wires

Application of the WFM technique for solving the scattering problem relies on a real space representation of the Kohn-Sham Hamiltonian and the wave functions. An efficient implementation based upon a high-order finite-difference scheme is discussed in Ref. [15]. In general, finite-difference schemes are suitable for treating systems with little symmetry. They have a computational efficiency that is comparable to that of plane wave basis set representations [44–47].

Similar to Eq. 2 we put the wave function ψ and the Kohn-Sham one-electron potential V on an equidistant grid in real space $\mathbf{r} = (x_j, y_k, z_l)$, where $x_j = x_0 + jh_x, y_k = y_0 + kh_y, z_l = z_0 + lh_z$ and h_x, h_y, h_z are the grid spacings in the x, y and z directions, respectively. It is computationally advantageous to replace the first order finite difference approximation (FDA) of Eq. 2 by a more general, high order FDA. For the x part this gives

$$\frac{\partial^2\psi(x_j, y_k, z_l)}{\partial x^2} \approx \frac{1}{h_x^2}\sum_{n=-N}^{N} c_n\psi(x_{j+n}, y_k, z_l), \tag{80}$$

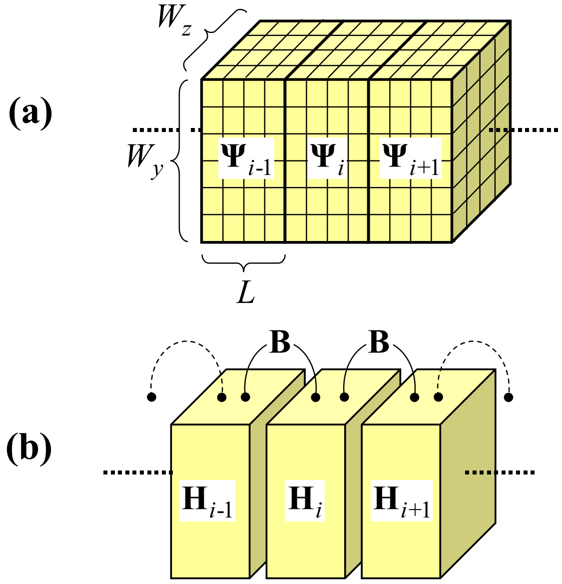

Figure 8: (a) The system is divided into cells indicated by an index i. The cells have $L \cdot W_y \cdot W_z$ grid points in the x, y and z directions, respectively. $\mathbf{\Psi}_i$ is the supervector that contains the wave function values on all grid points in cell i. (b) $\mathbf{H}_i$ is the Hamilton matrix connecting grid points within cell i; the $\mathbf{B}$-matrix connects grid points between neighboring cells and is independent of i.

with similar expressions for the y and z parts. Expressions for the coefficients c_n for various values of N are tabulated in Ref. [45]. The simplest approximation in Eq. (80) ($N = 1$, where $c_1 = c_{-1} = 1$ and $c_0 = -2$) reduces it to the three-dimensional equivalent of Eq. 2. However, in Ref. [15] it is demonstrated that the scattering problem can be solved much more efficiently using higher order FDA's with $N =$ 4-6.

In a FDA the Kohn-Sham equation becomes

$$(E - V_{j,k,l})\,\psi_{j,k,l} + \sum_{n=-N}^{N} \left(t_n^x \psi_{j+n,k,l} + t_n^y \psi_{j,k+n,l} + t_n^z \psi_{j,k,l+n}\right) = 0, \tag{81}$$

where $V, \psi_{j,k,l}$ is a shorthand notation for $V, \psi(x_j, y_k, z_l)$ and $t_n^{x,y,z} = \hbar^2/2mh^2_{x,y,z} \times c_n$. In order to make a connection to the formalism explained in the previous section, we divide the wire into cells of dimension $a_x \times a_y \times a_z$. The direction of the wire is given by the x-axis. The number of grid points in a cell is $L = a_x/h_x$, $W_y = a_y/h_y$, $W_z = a_z/h_z$ for the x, y and z directions respectively. The values $\psi_{j,k,l}$ where the indices j, k, l correspond to a single cell i are grouped into a supervector $\mathbf{\Psi}_i$. The idea is shown in Fig. 8. This supervector has the dimension $N_{\text{rs}} = L \cdot W_y \cdot W_z$, which is the total number of real space grid points in a cell. If we let i denote the position of the cell along the wire then Eq. (81) can then be rewritten as

$$-\mathbf{B}\mathbf{\Psi}_{i-1} + (E\mathbf{I} - \mathbf{H}_i)\mathbf{\Psi}_i - \mathbf{B}^\dagger \mathbf{\Psi}_{i+1} = 0, \tag{82}$$

for $i = -\infty, \ldots, \infty$. Here $\mathbf{I}$ is the $N_{\text{rs}} \times N_{\text{rs}}$ identity matrix. The matrix elements of the $N_{\text{rs}} \times N_{\text{rs}}$ matrices $\mathbf{H}_i$ and $\mathbf{B}$ can be derived straightforwardly from Eq. (81). The expressions are given in Ref. [15]. Clearly Eq. 82 is the same as Eq. 62, which means that we can use the WFM method to solve the scattering problem.

As a first step, the one-electron self-consistent potentials of the bulk leads and the scattering region containing the wire are obtained from DFT calculations. Subsequently the scattering problem is solved at the Fermi energy by matching the modes in the leads to the wave function in the scattering region.

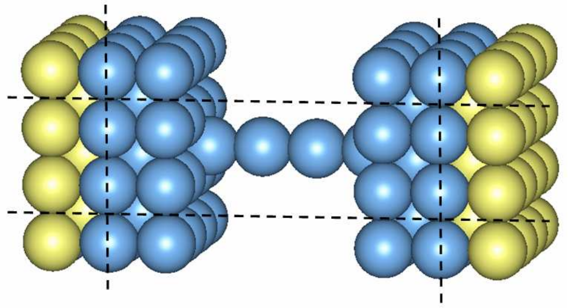

Figure 9: Structure of an atomic wire consisting of two sodium atoms between two sodium leads terminated by (001) surfaces. The boundaries of the supercell are indicated by dashed lines. Bulk atoms are indicated by yellow (light grey) balls and atoms in the scattering region by blue (dark grey) balls, respectively.

2.1 Conductance of monatomic sodium wires

Conductors whose cross section contains only a small number of atoms are commonly called "atomic wires". Clear evidence that the fundamental limit of a one atom cross section can be reached, has been presented for gold atomic wires [48, 49]. Over the last decade the electronic transport in atomic wires made of various metals has been characterized in great detail experimentally [50–52]. Such wires have conductances of the order of the quantum unit $G_0 = 2e^2/h$.[9] Atomic wires that have a cross section of just one atom, so-called "monatomic" wires, are the ultimate examples of quasi-one-dimensional systems. Here the effects of a reduced dimensionality are expected to be most pronounced. One of the most striking features of monatomic wires is the non-monotonic behavior of the conductance as a function of the number of atoms in the wire [53,54]. In particular, the conductance in such wires oscillates. For simple monovalent metals the oscillation has a period that corresponds to two atoms, i.e. the conductance of wires consisting of an odd number of atoms is different from that of even numbered wires. The amplitude of such oscillations is of order $0.1\ G_0$. The central questions are: what determines the phase and amplitude of the oscillation and how robust are these with respect to changes in the geometry of the wire and in the coupling between the wire and the leads?

From our first-principles calculations on sodium monatomic wires we find that odd numbered wires always have a conductance close to $1\ G_0$ and that this value is not very sensitive to changes in the geometry or in the coupling [32]. Even numbered wires have lower conductances, whose values are determined by the geometry and the coupling. This general pattern can be understood from the electronic levels of free-standing wires giving rise to transmission resonances. We analyze our first-principles results using a simple tight-binding model. In particular, we show that local charge neutrality of the sodium wires provides a strong constraint on the phase of the conductance oscillation. In absence of a significant charge transfer between the wire and the leads, a transmission resonance is pinned at the Fermi energy for wires containing an odd number of atoms, which leads to a conductance close to one quantum unit. Obtaining quantitative values for the conductance of even-numbered wires in particular, requires well-converged first-principles calculations using a realistic structure of the wire and the leads.

The one-electron potentials of the leads and the scattering regions are extracted from two self-consistent DFT calculations for bulk bcc sodium and for the supercell shown in Fig. 9, respectively, using a standard approach based upon normconserving pseudopotentials and a plane wave basis set. It turns out that, in order to obtain potentials that are converged, the total energies in such self-consistent calculations have to be converged to within 5×10^{-7} Hartrees. One assumes that the leads outside the scattering region

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[9] The factor of 2 with respect to Eq. 1 results from spin degeneracy.

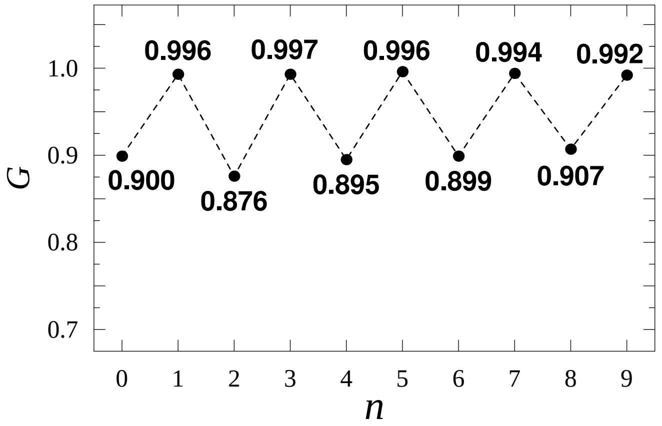

Figure 10: Conductance (in units of G_0) as a function of the number of atoms in the atomic chain. All atomic bond lengthes in the system are equal to the bulk value $d = 6.91a_0$.

consist of bulk material. This means that at the edges of the scattering region, the potential should join smoothly to the potentials of the bulk leads. We have checked that this is the case. Enlarging the scattering region by including two extra atomic layers in each lead changes the results reported for the conductance only by $\sim 1.5\%$ for even-numbered wires and $\lesssim 0.5\%$ for odd-numbered wires. The Fermi energy is extracted from the bulk calculation [15]. The only parameters in calculating the conductance within the finite-difference scheme are the order N of the finite-difference approximation of the kinetic energy (i.e., the second derivative) and the spacing $h_{x,y,z}$ between the real-space grid points. We use $N = 4$ and $h_{x,y,z} = 0.80a_0$; for details and convergence tests we refer to Ref. [15]. The total transmission is averaged over a 8×8 $\mathbf{k}_{\|}$-point grid in the lateral BZ of the supercell. Most calculations are done for a 2×2 lateral supercell. Enlarging the supercell changes the conductance only marginally as discussed in Ref. [32].

The electron transport in the crystalline leads is ballistic, i.e. an electron goes through the leads without any scattering. The transport properties of a monatomic wire suspended between two leads depend upon three factors; the number of atoms in the chain, the geometry of the wire, and the contact between wire and leads.

The calculated conductance as a function of the number of atoms in the atomic chain is given in Fig. 10. Since a sodium atom has valence one, both the infinite sodium chain and bulk sodium have a half-filled band, and the infinite wire has one conducting channel at the Fermi level. The conductance of the infinite chain is equal to the quantum unit G_0, and the conductance of finite wires is $\leq G_0$. As can be observed in Fig. 10 the conductance exhibits a regular oscillation as a function of the number of atoms in the wire. The conductance is very close to G_0 for odd-numbered wires, and for even-numbered wires it is $\sim 10\%$ lower. Such a behavior of the conductance in atomic-sized conductors is very different from ohmic behavior in macroscopic conductors; it expresses the quantum nature of the electron transport at the nanoscale.

In order to interpret the even-odd oscillation we have calculated the conductance as a function of energy for wires of different length. The results for monatomic wires consisting of four and five atoms are shown in Fig. 11. Resonant peaks in the conductance can be clearly identified. Qualitatively they correspond to energy levels of a free-standing Na wire, which are shifted and broadened into resonances by the interaction of the wire with the leads. To illustrate this, the calculated energy levels of free-standing wires of four and five atoms are shown as bars in Fig. 11. The levels are sufficiently close to the resonant energies to warrant an interpretation of the conductance in terms of a transmission through levels of the

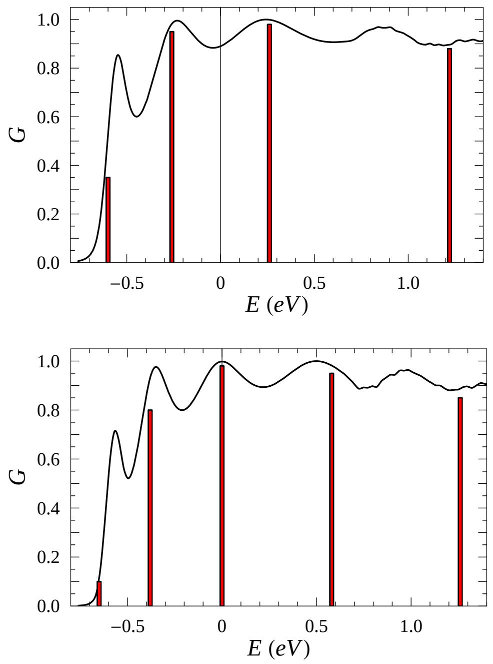

Figure 11: Conductance (in units of G_0) as a function of energy for monatomic wires consisting of four (top figure) and five (bottom figure) atoms. The red (grey) bars correspond to the energy levels of free-standing wires. $E = 0$ corresponds to the Fermi level.

wire. As is clearly observed in Fig. 11, the Fermi level is in between two resonant peaks for a four atom wire and right on top of a resonance for a five atom wire. By calculating the conductance as a function of energy for wires of different length it can be shown that this observation can be generalized. The Fermi level is between resonances for even-numbered wires and on top of a resonance for odd-numbered wires.

2.1.1 Simple tight-binding model

To support the intuitive picture presented in the previous section we use a simple tight-binding model as shown in Fig. 12, in which the leads are modeled as quasi-one-dimensional systems described by effective parameters. Here ε_0, β are the on-site energies and nearest neighbor hopping coefficients of the leads, and ε_0', β' are the corresponding parameters of the wire. The coupling between the left (right) electrode and the atomic chain is given by the hopping coefficient β_c (β_c').

If the system has mirror symmetry, the coupling is symmetric, i.e. $\beta_c = \beta_c'$. The leads and the chain are made of the same material (sodium). If one assumes that all atoms are neutral (local charge neutrality), then it is not unreasonable to set $\varepsilon_0 = \varepsilon_0'$. The conductance can be calculated analytically for this model using WFM [27]. The parameter β can be used as a scaling parameter. In the following all energy parameters $\varepsilon_0, \varepsilon_0', \beta', \beta_c, \beta_c'$ are in units of β. The conductance of a wire at the Fermi energy consisting of n atoms is given by

$$\begin{aligned} G &= G_0, && n\,\text{odd} \\ &= G_0\,\frac{4\,\beta_c^4/\beta'^2}{\left[1+\beta_c^4/\beta'^2\right]^2}, && n\,\text{even}. \end{aligned} \tag{83}$$

The conductance for odd-numbered wires is equal to the quantum unit, and it is smaller than the quantum unit for even-numbered wires (unless by accident $\beta_c^2 = \beta'$).

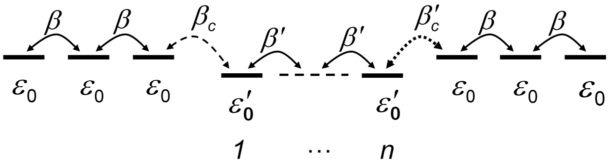

Figure 12: Tight-binding representation of the n-atomic wire attached to two semi-infinite one-dimensional leads.

It is instructive to study some other consequences of the tight-binding model. If $\Delta\varepsilon = \varepsilon_0 - \varepsilon_0' \neq 0$ then a charge transfer will take place between the leads and the wire. The conductance calculated at the Fermi energy for a one-site wire ($n = 1$) and a two-site wire ($n = 2$) become, respectively,

$$G = G_0 \frac{4\beta_c^4}{\Delta\varepsilon^2 + 4\beta_c^4}, \tag{84}$$

$$G = G_0 \frac{4\beta_c^4 \beta'^2}{\left[\beta_c^4 + (\beta' + \Delta\varepsilon)^2\right]\left[\beta_c^4 + (\beta' - \Delta\varepsilon)^2\right]}. \tag{85}$$

According to Eq. (84) a nonzero $\Delta\varepsilon$ suppresses the transmission through a one-site wire. The transmission is shifted "off resonance" and the conductance becomes smaller than the quantum unit. However, the coupling between wire and lead also causes a broadening of the resonance, which is proportional to β_c. This broadening partially compensates for the decrease of the conductance. If the coupling is sufficiently strong, i.e. $4\beta_c^4 \gg \Delta\varepsilon^2$, then the conductance is again close to the quantum unit. In the limit of weak coupling, i.e. $4\beta_c^4 \ll \Delta\varepsilon^2$, the conductance goes to zero with decreasing β_c for any nonzero $\Delta\varepsilon$.

The conductance of a two-site wire, see Eq. (85), behaves qualitatively different as a function of the coupling strength β_c. In the weak coupling limit, i.e. $\beta_c^4 \ll (\beta' \pm \Delta\varepsilon)^2$ the conductance goes to zero with decreasing β_c and the decrease is faster than for a one-site wire. Note that this only holds for $\Delta\varepsilon \ll \beta'$. If $\Delta\varepsilon \sim \beta'$ then the conductance decreases more slowly with decreasing β_c for a two-site wire than for a one-site wire. If the coupling between wire and lead is strong, i.e. $\beta_c^4 \gg (\beta' \pm \Delta\varepsilon)^2$, then the conductance always decreases with increasing β_c. This is due to a phenomenon called "pair annihilation" of resonances [55], which happens if the resonance widths become larger than the spacing between the resonances. Between the strong and weak coupling regimes there is a value of β_c (close to 1) where the conductance of a two-site wire is equal to the quantum unit.

The conductance of longer wires, i.e. $n > 2$, can be interpreted along the same lines. For small $\Delta\varepsilon$, the odd-numbered wires resemble the one-site wire and the even-numbered wires resemble the two-site wire. For a very large range of coupling strengths β_c one obtains an even-odd oscillation in the conductance of a nearly constant amplitude. The conductance of odd-numbered chains is close to the quantum unit and that of even-numbered chains is smaller by an amount that depends upon the coupling between wire and lead. Apparently, this is the case that corresponds to the results of our first-principles calculations, see Fig. 10. If $\Delta\varepsilon$ becomes larger, the conductance of all wires as a function of β_c becomes qualitatively similar to that of the two-site wire. The amplitude and even the phase of the conductance oscillation as a function of the wire length then strongly depends upon the coupling β_c of the wire to the lead. Note that if $\Delta\varepsilon$ is significant, it will be accompanied by a significant charge transfer between wire and leads. In our first-principles calculations we have found no indication of such a large charge transfer.

In conclusion, odd-numbered wires have a conductance close to the quantum unit $G_0 = 2e^2/h$ and even-numbered wires have a lower conductance. This oscillation is remarkably robust, as we show by systematically varying the structure of the wires and the geometry of the contacts between the wires and the electrodes. The phase of the oscillation is not affected by these structural variations. The conductance of even-numbered wires is sensitive to the wire geometry. Increasing the interatomic distances in the wire and/or strengthening the contacts between wire and leads increases the conductance of even-numbered wires; increasing the asymmetry between the interatomic distances or between left and right contacts decreases the conductance.

3 TB-MTO implementation: layered (magnetic) structures

A computational scheme suitable for studying microscopic transport in layered magnetic materials needs to be able to describe the complex electronic structures characteristic of ($3d$) transition metal elements. In addition, it should be possible to model layered systems with different lattice parameters and to model disorder; we do this using large lateral supercells. The Local Spin-Density Approximation (LSDA) of DFT is the appropriate framework for treating itinerant electron systems from first-principles [56].

Oscillatory exchange coupling in layered magnetic structures was discussed by Bruno in terms of generalized reflection and transmission matrices [57] which were calculated by Stiles [58,59] for realistic electronic structures using a scheme [1, 2] based on linearized augmented plane waves (LAPWs). At an interface between a non-magnetic and a magnetic metal, the different electronic structures of the majority and minority spin electrons in the magnetic material give rise to strongly spin-dependent reflection [60, 61]. Schep *et al.* used transmission and reflection matrices calculated from first-principles with an embedding surface Green function method [62] to calculate spin-dependent interface resistances for specular Cu|Co interfaces embedded in diffusive bulk material [3]. The resulting good agreement with experiment indicated that interface disorder is less important than the spin-dependent reflection and transmission from a perfect interface. Calculations of domain wall resistances as a function of the domain wall thickness illustrated the usefulness of calculating the full scattering matrix [4, 63]. However, the LAPW basis set used by Stiles and Schep was computationally too expensive to allow repeated lateral supercells to be used to model interfaces between materials with very different, incommensurate lattice parameters or to model disorder. This is true of all plane-wave based basis sets which typically require of order 100 plane waves per atom in order to describe transition metal atom electronic structures reasonably well.

Muffin-tin orbitals (MTO) form a flexible, minimal basis set leading to highly efficient computational schemes for solving the Kohn-Sham equations of DFT [33,64,65]. For the close packed structures adopted by the magnetic materials Fe, Co, Ni and their alloys, a basis set of 9 functions (s, p, and d orbitals) per atom in combination with the atomic sphere approximation (ASA) for the potential leads to errors in describing the electronic structure which are comparable to the absolute errors incurred by using the LSDA. The tight-binding linearized muffin tin orbital (TB-LMTO) surface Green function (SGF) method was developed to study the electronic structure of interfaces and other layered systems. When combined with the coherent-potential approximation (CPA), it allows the electronic structure, charge and spin densities of layered materials with substitutional disorder to be calculated self-consistently very efficiently [66]. MTOs thus satisfy our requirements of being able to treat complex electronic structures efficiently.

To combine the WFM method with muffin-tin orbitals, it turns out to be convenient to use the so-called "tail-cancellation" condition[10]

$$\sum_{R',l'm'} \left[P^{\alpha}_{Rl}(\varepsilon)\delta_{RR'}\delta_{ll'}\delta_{mm'} - S^{\alpha}_{Rlm;R'l'm'}\right] c^{\alpha}_{R'l'm'} = 0, \tag{86}$$

in terms of potential functions $P^{\alpha}_{Rl}(\varepsilon)$ which characterize the AS potentials and the potential-independent

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[10] This equation is nothing other than the KKR equation in the ASA in which the kinetic energy in the interstitial region is taken to be zero and the volume of the interstitial region is made to vanish by replacing the muffin tin spheres with space-filling atomic spheres. This choice leads to structure constants which are energy and scale independent, unlike the KKR structure constants. The potential function $P_l(\varepsilon)$ is simply related to the logarithmic derivative $D_l(\varepsilon)$ as $P_l(\varepsilon) = 2(2l+1)(D_l(\varepsilon)+l+1)/(D_l(\varepsilon)-l$.

screened structure constant matrix $S^{\alpha}_{Rlm;R'l'm'}$ whose range in real space depends on a set of screening parameters $\{\alpha_l\}$. The set of parameters which minimize the range of hopping is denoted $\alpha = \beta$. The equation analogous to Eq. (62) which we use to solve the scattering problem is then

$$-\mathbf{S}^{\beta}_{i,i-1}\mathbf{c}_{i-1} + \left(\mathbf{P}^{\beta}_{i,i}(\varepsilon) - \mathbf{S}^{\beta}_{i,i}\right)\mathbf{c}_i - \mathbf{S}^{\beta}_{i,i+1}\mathbf{c}_{i+1} = 0. \tag{87}$$

$\mathbf{c}_i$ is a $(l_{\max}+1)^2 N \equiv M$ dimensional vector consisting of the coefficients of the i-th layer $c_{i,Rlm}$ with N atomic sites R and $(l_{\max}+1)^2$ orbitals lm per site.

In the actual calculation of the transmission matrix, we adopt the following procedure. First of all two separate self-consistent field calculations are performed for the left and right leads making use of their lattice periodicity to calculate the electron densities (for magnetic materials, the spin-densities) as well as corresponding Fermi energies. Next, a self consistent field calculation is carried out for the scattering region between the leads subject to the requirement that the Fermi energies in the right- and left-hand leads are equal. We now have a charge (spin) density in all space as well as the corresponding Kohn-Sham effective potential and can proceed to the solution of the transport problem.

Even though the theoretical scheme outlined above contains no adjustable parameters, its practical implementation does involve approximations, which need to be evaluated. We illustrate the formalism sketched in the previous section by calculating the transmission matrix for planar interfaces. We begin by studying ideal ordered interfaces (3.1), then describe how interface disorder can be modeled using large lateral supercells and the results analyzed using "channel decomposition" (3.2).

3.1 Ordered Interfaces

A recurring theme in condensed matter physics in the last twenty years has been the discovery of new physical effects and properties in systems with reduced dimensions; the prospect of exploiting these effects and properties in logical processing, sensing and storage devices is an important driving force behind nano-science and -technology. In semiconductors, the electronic structures of the electrons responsible for conduction can be described using simple models. The same is not true of the ferromagnetic transition metals which form the basis for magnetoelectronics. It is the non-trivial spin-dependence of the transmission and reflection of electrons at magnetic interfaces which provides the key to understanding phenomena such as oscillatory exchange coupling, giant- and tunneling- magnetoresistance, spin transfer torque, spin-pumping and spin injection [67]. For well-studied material combinations such as Co|Cu and Fe|Cr, modest spin-dependence of the interface transmission [3, 7, 68] of the order of 10-20% is sufficient to account for experimental observations [69].

However, the confrontation of theory and experiment just referred to is at best indirect and model-dependent. Even though the theory of transport in small structures is formulated in terms of transmission and reflection matrices [30], measuring interface transparencies directly has proven quite difficult [70]. To identify interfaces suitable for experimental study, we undertook [35] a systematic materials-specific study of the orientation dependence of the interface transmission between pairs of isostructural metals whose lattice constants match within a percent or so in the hope that it will prove possible to grow such interfaces epitaxially.

3.1.1 Al|Ag

One of the metal pairs we studied was Al|Ag. Both metals have the fcc crystal structure and their lattice constants are matched within 1%. Aluminium is a textbook [71] example of a system well described by the (nearly) free electron model. Silver, also usually assumed to be a free electron-like material, is a noble metal with high conductivity which is frequently used for electrical contacting. We found that in spite of the simplicity of both metals' electronic structures the transmission through Al|Ag interfaces can differ quite significantly from the predictions of the free electron model. In particular, between (111) and (001) orientations we find a factor 2 difference in interface transmission for clean Al|Ag interfaces. For free electrons the anisotropy should vanish. Our result is insensitive to interface disorder. We identify a new factor responsible for this difference which is not related to the standard velocity- [72, 73] or symmetry-mismatch [34, 39] mechanisms.

A free electron description of interface scattering, in which the effect of the crystal potential on transport is completely neglected, underlies the Blonder-Tinkham-Klapwijk or BTK theory [74] used to interpret [72, 73] Andreev reflection (AR) experiments. Point contact AR experiments are increasingly used to identify the pairing symmetry of superconductors and, in the field of magnetoelectronics, to determine the polarization of magnetic materials [75, 76]. Our finding that the electronic structure can have such a large effect on the interface transmission, implies that experiments should be analyzed using more sophisticated models.

Our study was based upon first-principles calculations of the interface electronic structure performed within the framework of density functional theory (DFT) and the local spin density approximation (LSDA). Bulk and interface potentials were determined self-consistently using the tight binding linearized muffin tin orbital (TB-LMTO) [65] surface Green's function method [66]. We assumed common lattice constants for both metals of a given structure e.g. $a_{Al} = a_{Ag} = 4.05$ Å. The potentials obtained in this way were used as input to the TB-MTO wave function-matching [7, 34] calculation of the transmission and reflection coefficients between Bloch states on either side of the interface. For disordered systems, the ASA potentials were calculated using the layer CPA (coherent potential approximation). For the scattering matrix calculation, disorder was modeled using large lateral supercells in which the CPA-ASA potentials were distributed at random in the appropriate concentrations The results of the calculations for a number of lattice-matched materials are summarized in Table 3.1.1.

The Sharvin conductances, G_A and G_B, reported in the third and fourth columns of Table 3.1.1 are proportional to the number of states at the Fermi level propagating in the transport direction. They are properties of the bulk materials which are determined by the area of the Fermi surface projections and are a measure of the current-carrying capacity of the conductor in the ballistic regime. The largest intrinsic orientation dependence, seen to be about 13 %, is found for Mo; for Al and Ag, respectively, it is less than 8% and 5%.

The interface transmission in column five of Table 3.1.1 is expressed as a conductance, $G_{A|B} = e^2/h \sum_{\mu\nu} T_{\mu\nu}$, where $T_{\mu\nu}$ is the probability for the incoming state ν in material A to be transmitted through the interface into the outgoing state μ in material B. For most pairs of materials[11], the orientation dependence of $G_{A|B}$ is modest ($\sim$ 15% for Mo|W) and the interface conductance itself tends to be slightly smaller than the lower of the two Sharvin conductances. For these systems the behavior of the transmission appears to be determined by the projection of the Fermi surfaces. However, this is not so for Al|Ag and Al|Au interfaces. Here we observe a large anisotropy in the transport properties. The factor 2 difference in transmission between (111) and (001) orientations[12] results in a factor 4 difference between interface resistances estimated using the method of [3, 7].

The transmission probability for the (111) and (001) orientations is plotted in Figs. 13c and 13f as a function of the wave-vector component parallel to the interface, $\mathbf{k}_{\|}$, within the 2D interface Brillouin zones (BZ). A qualitative difference between the two orientations can be observed. In the (111) case, the

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[11] Fe/Cr is an exception. For the majority spin channel, a large orientation dependence of the interface tranmission is predicted. Unlike in the case of Al/Ag, this result is very sensitive to interface disorder. In addition, a single spin channel cannot be studied directly making it difficult to obtain an unambiguous experimental result.

[12] We performed an extensive series of total energy calculations using LDA and GGA approximations to relax the various Al/Ag interfaces. Only a small dependence of the interface energy on the orientation was found. The transport calculations were repeated using the resulting relaxed geometries. The effect on the interface transmission is less than 3% which is negligible on the scale of the predicted factor of two orientation dependence.

A|B		G_A	G_B	$G_{A\|B}$	$2SR$
Al|Ag	(111)	0.69	0.45	0.41 (0.36)	0.64 (0.92)
a$_{fcc}$ = 4.05 Å	(110)	0.68	0.47	0.30 (0.32)	1.60 (1.39)
	(001)	0.73	0.45	0.22 (0.24)	2.82 (2.37)
Al|Au	(111)	0.69	0.44	0.41 (0.35)	0.60 (0.99)
a$_{fcc}$ = 4.05 Å	(001)	0.73	0.46	0.24 (0.26)	2.37 (2.14)
Pd|Pt	(111)	0.62	0.71	0.55 (0.54)	0.30 (0.33)
a$_{fcc}$ = 3.89 Å	(001)	0.58	0.70	0.52 (0.51)	0.37 (0.39)
W|Mo	(001)	0.45	0.59	0.42 (0.42)	0.42 (0.42)
a$_{bcc}$ = 3.16 Å	(110)	0.40	0.54	0.37 (0.38)	0.52 (0.47)
Cu|Co	(111)*	0.56	0.47	0.43 (0.43)	0.34 (0.35)
majority	(001)	0.55	0.49	0.46 (0.45)	0.26 (0.27)
a$_{fcc}$ = 3.61 Å	(110)	0.59	0.50	0.46 (0.46)	0.35 (0.35)
Cu|Co	(111)*	0.56	1.05	0.36 (0.31)	1.38 (1.82)
minority	(001)	0.55	1.11	0.32 (0.32)	1.79 (1.79)
a$_{fcc}$ = 3.61 Å	(110)	0.59	1.04	0.31 (0.35)	1.89 (1.55)
Cr|Fe	(111)	0.61	0.82	0.27 (0.31)	2.22 (1.84)
majority	(001)	0.64	0.82	0.11 (0.25)	7.46 (2.55)
a$_{bcc}$ = 2.87 Å	(110)	0.59	0.78	0.22 (0.27)	3.04 (2.18)
Cr|Fe	(111)	0.61	0.41	0.34 (0.34)	0.93 (0.95)
minority	(001)	0.64	0.46	0.35 (0.35)	0.98 (0.95)
a$_{bcc}$ = 2.87 Å	(110)*	0.59	0.40	0.32 (0.32)	1.03 (1.06)

Table 1: Sharvin conductances and interface transmissions in units of $10^{15}\Omega^{-1}m^{-2}$, interface resistances SR [3,7] for ideal (and, in brackets, for disordered) interfaces in units of $10^{-15}\Omega m^2$. S is the area of the sample for which R is measured. Interface disorder was modeled in 10×10 lateral supercells with two layers of 50-50 alloy. The largest uncertainty between different configurations of disorder is about 2.3%. The values given are for a single spin. For the pairs of materials and orientations indicated by a (*), comparison of the interface resistances shown in the last two columns with experimental values extracted from measurement on [3, 7, 34].

transmission is almost uniformly high wherever there are states on both sides of the interface. The (001) orientation exhibits more variation with high transmission in the central and outer regions of the 2D BZ but much lower in a ring-shaped region in between. The presence of this "cold ring" is the reason why the total transmission is lower for the (001) orientation. Explaining the transparency anisotropy of Al|Ag interfaces requires finding an explanation for the low transmission values in this region of the 2D BZ.

Two mechanisms are usually taken into account when analyzing the scattering at perfect interfaces. The first, velocity mismatch, is the modulation of the transmission by a factor reminiscent of the free electron formula for the transmission through a potential step: $T = 4v_L v_R/(v_L + v_R)^2$ where $v_{L/R}$ are the components of the Fermi velocities in the transport direction on the left and right sides of the interface. This modulation is indeed present in our calculated transmissions but its effect tends to be noticeable only when one of the velocities is almost vanishingly small. Naive application of the free electron formula yields uniformly good transmission[13]independent of the orientation. Symmetry mismatch, the second

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[13] Morover the free electron formula would lead to the violation of the unitarity of the scattering matrix (*i.e.*

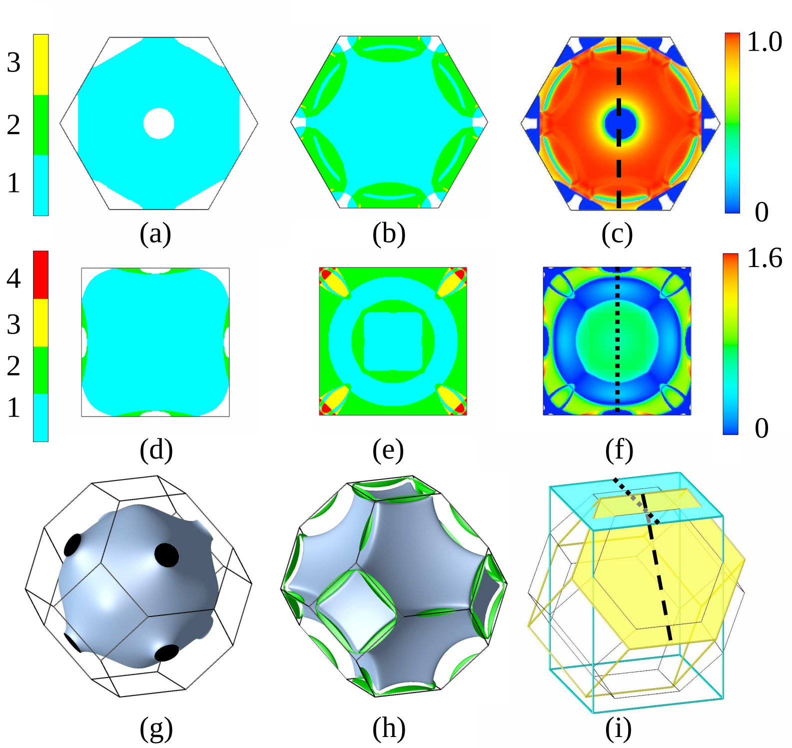

Figure 13: Top row: Fermi surface projections for (a) Ag, (b) Al and (c) transmission probabilities in 2DBZ for (111) orientation. Middle row: Same for (001) orientation. The color bars on the left indicate the number of scattering states in the leads for a given two dimensional wave vector $\mathbf{k}_{\|}$. The transmission probabilities indicated by the color bars on the right can exceed 1 for $\mathbf{k}_{\|}$s for which there is more than one scattering state in both Ag and Al. Bottom row: Fermi surfaces of (g) Ag and (h) Al, (i) the interface adapted BZ for (001) and (111) orientations. The vertical dashed line in (c) and on the yellow plane in panel (i) indicate the cross-section used in the left-hand panel of Fig. 14 while the vertical dotted line in (f) and on the blue plane in panel (i) indicate the cross-section used in the right-hand panel.

mechanism, can suppress the transmission between states of incompatible symmetries (*e.g.* even vs. odd etc.). Examination of the eigenvectors demonstrates that this is not the case for the Al|Ag system. For example, states on both sides of the interface, with $\mathbf{k}_{\|}$ along the vertical dotted line in Fig. 13f, are even under reflection in the plane defined by this line and the (001) transport direction. Their orbital composition (s,p_y,p_z,d_{yz},$d_{3z^2-r^2}$,$d_{x^2-y^2}$ where the y axis is parallel to the dotted line and z is the transport direction) is essentially the same for both materials. The same holds for states along other symmetry lines/planes and general $\mathbf{k}_{\|}$ points (in the sense of orbital composition). The origin of the "cold ring" must be sought elsewhere.

In spite of the failure of the free electron transmission formula, this simple model serves as a useful starting point for analyzing the Fermi surface (FS) topologies. In the simplest possible approach, we model the FS of Ag (shown in Fig. 13g) as a sphere which fits into the first BZ. A larger sphere, accommodating three electrons, is needed for trivalent Al. In an extended zone scheme, conservation of momentum parallel to the interface dictates that the transmission through a specular interface is non-zero only between states with the same values of $\mathbf{k}_{\|}$; these are the $\mathbf{k}_{\|}$-vectors belonging to the region where projections of the Fermi spheres on a plane perpendicular to the transport direction overlap. For systems with lattice periodicity, we must use a downfolded FS, with fragments of the original FS sphere back-translated into

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the conservation of particles) whenever there is more than one state on either side of the interface.

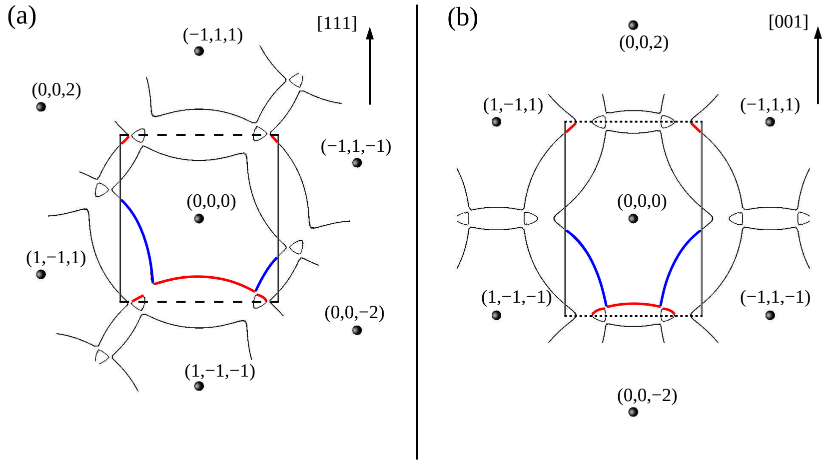

Figure 14: Intersection of a (110) plane with the Al Fermi surface and with the interface adapted BZs indicated in Fig. 13i (where the meaning of the dashed and dotted lines is explained). The labeled dots indicate the positions of the RL sites with coordinates given in units of $2\pi/a$. The red (blue) lines indicate regions of high (low) transmission.

the 1st Brillouin zone, a procedure which can be realized geometrically by placing spheres accommodating three electrons on reciprocal lattice (RL) sites and then only considering the fragments in the first BZ. Examination of the FS of Al calculated from first-principles (Fig. 13h) and its cross-section (Fig. 14) reveals that, in spite of its apparent complexity, it remains essentially (piecewise) spherical. For some values of $\mathbf{k}_{||}$ (see Figs. 13b and 13e), Al can now have more than one propagating state. Nevertheless, in the free electron limit, the downfolded states are strictly orthogonal to the states in Ag and the total transmission is unchanged. For a reduced zone scheme, we formulate the following rule: *The transmission between states in two (nearly) free electron materials which have the same* $\mathbf{k}_{||}$*, but originate from reciprocal lattice sites whose parallel components* do not *coincide, vanishes in the free electron limit and is expected to be strongly suppressed for nearly free electron like materials.*

Obviously, the truly free electron system can not exhibit anisotropy. However, in the presence of the periodic potential the original, piecewise-spherical Fermi surface and consequently the transmission is going to be modified. Firstly, since the wave functions are no longer pure plane waves, the strict orthogonality of the downfolded states is relaxed and the transmission can assume finite although typically small values (hence *suppressed* instead of *zero* in the above rule). Secondly, the shape of the Fermi surface changes with the modifications being strongest in the vicinity of RL planes where, for Al, we observe the opening of gaps between previously connected fragments. The anisotropy is mostly related to this second effect.

In Fig. 14, we show the intersection of the Al FS with a (110) plane. The two plots are rotated so that the vertical axis in Fig. 14a is the [111] direction while in Fig. 14b it is [001]. In both cases the positions of the nearest RL sites (on which spheres are centered) are shown together with the cross-section through the relevant interface-adapted Brillouin zone, which is different for each orientation; see Fig. 13i. We can now readily identify spheres from which various fragments of the Fermi surface originate and mark those fragments with positive (upward) velocities, according to the rule given above, as having high (red) or low (blue) transmissions. In the (001) case, the "high" fragments originate from (0,0,0) and (0,0,-2) centered spheres. Comparing Figs. 13f and 14b, we note that the position of the gaps opened between these spheres by Bragg reflection on the (001) and $(00\bar{1})$ planes coincides, in projection along the [001] direction, with the position of the "cold ring" in Fig. 13f. The other states present in this region originate from (1,-1,-1) (and equivalent) centered spheres, are therefore nearly orthogonal to states in Ag centered on (0,0,0) and so have low transmission. In the (111) case however, the large fragments of FS belonging to the same (1,-1,-1) sphere have high transmissions (Fig. 14a) and dominate transport. In addition, the

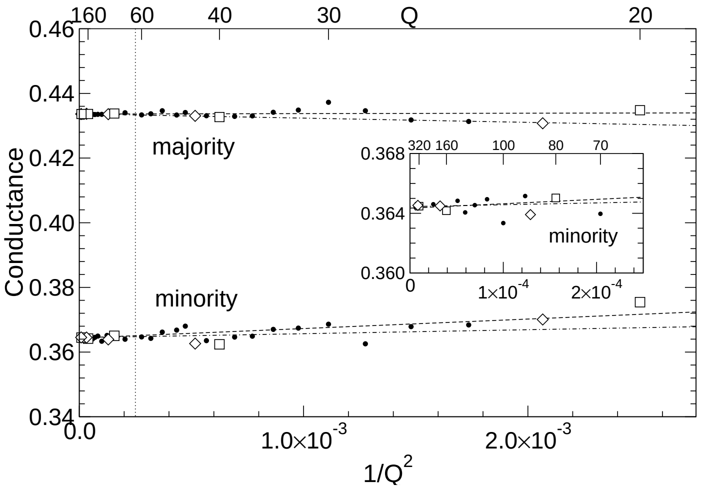

Figure 15: Interface conductance $G^{\sigma}(111)$ (in units of $10^{15}\ \Omega^{-1}\mathrm{m}^{-2}$) for an *fcc* Cu|Co(111) interface for majority and minority spins plotted as a function of the normalized area element used in the Brillouin zone summation, $\Delta^2\mathbf{k}_{\|}/A_{BZ} = 1/Q^2$. Q, the number of intervals along the reciprocal lattice vector is indicated at the top of the figure. The dashed line is the weighted (weighting Q^2) least-squares fit to the series $Q = 20, 40, 80, 160, 320$ shown as squares; the dash-dotted line is the weighted least-squares fit to the series $Q = 22, 44, 88, 176, 352$ shown as diamonds. The part of the curve for the Co minority spin case to the left of the vertical dotted line is shown on an expanded scale in the inset. An *fcc* lattice constant of $a = 3.614\mathring{A}$ and von Barth-Hedin exchange correlation potential were used.

effect of gap-opening is reduced in this orientation because of the rotation. Combination of these two factors results in the almost uniformly high transmission seen in Fig. 13c.

We can now finally identify the origin of the transmission anisotropy for Al|Ag interface. It stems from two factors: (i) the near orthogonality of the downfolded Al states to those belonging to the simple Ag sphere and (ii) the gaps opened in the continuous free electron Fermi surface by the periodic potential. The latter factor is of course related to the symmetry of the underlying crystal lattice and directly responsible for the introduction of the orientation dependence. For Al|Au interfaces, the interface transmissions and resistances are very similar to the Al|Ag case. The predicted anisotropic interface resistance and Andreev reflection (not shown) are not very sensitive to interface disorder and should be observable experimentally.

3.1.2 Cu|Co (111)

Our starting point is a self-consistent TB-LMTO SGF calculation [66] for the interface embedded between semi-infinite Cu and Co leads whose potentials and spin-densities were determined self-consistently in separate "bulk" calculations. The charge and spin-densities are allowed to vary in n_{Cu} layers of Cu and n_{Co} layers of Co bounding the interface. In the Cu layers, only tiny moments are induced. Only four layers away from the interface on the Co side, the magnetic moments are very close to the bulk values. At the interface, where the d-bandwidth is reduced as a result of the lower coordination number, the moments are suppressed rather than enhanced.

Once the interface potential has been obtained, the transmission matrix can be calculated and the BZ summation carried out. The convergence of this summation, shown in Fig. 15 for a (111) interface, a lattice constant of $a = 3.614\mathring{A}$ and an *spd* basis, closely parallels the behavior found on calculating the Sharvin conductance of the leads and does not represent a limitation in practice. Converged values of

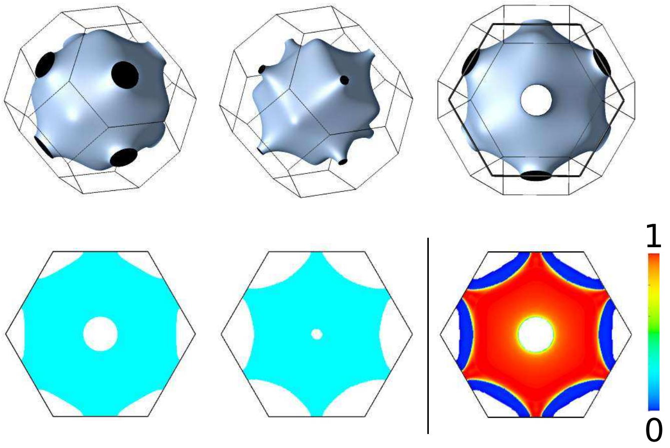

Figure 16: Top row, left-hand panel: Fermi surface (FS) of Cu; middle panel: majority-spin FS of Co; right-hand panel: Cu FS viewed along the (111) direction with a projection of the bulk fcc Brillouin zone (BZ) onto a plane perpendicular to this direction and of the two dimensional BZ. Bottom row, left-hand and middle panels: projections onto a plane perpendicular to the (111) direction of the Cu and majority-spin Co Fermi surfaces; right-hand panel: transmission probability for majority-spin states as a function of transverse crystal momentum, $T(\mathbf{k}_\parallel)$ for an *fcc* Cu|Co(111) interface.

the transmission probabilities

$$G^\sigma(\hat{n}) = \frac{e^2}{h} \sum_{m,n,\mathbf{k}_\parallel} T^\sigma_{mn}(\mathbf{k}_\parallel) = \frac{e^2}{h} \sum_{m,n,k_\parallel} |t^\sigma_{mn}(\mathbf{k}_\parallel)|^2 \tag{88}$$

are 0.434 and 0.364 in units of $10^{15}\,\Omega^{-1}\mathrm{m}^{-2}$ for majority and minority spins, respectively. The apparently modest spin-dependence of “bare” interface conductances ($\sim 20\%$) can lead to spin-dependent interface resistances differing by a factor of $\sim 3-5$. To obtain estimates of the interface resistance for highly transparent interfaces, the “bare” transmissions cannot be used. $R^{LB} = 1/G^{LB}$ results in a finite “interface” resistance, even for a fictitious interface between identical materials. Schep *et al.* [3] derived an expression for the resistance of transparent interfaces in terms of the interface transmission, which takes into account the finiteness of the conductance of the perfect leads:

$$R^{Schep}_\sigma(A|B) = \frac{h}{e^2}\left[\frac{1}{\sum T^\sigma_{mn}} - \frac{1}{2}\left(\frac{1}{N^\sigma_A} + \frac{1}{N^\sigma_B}\right)\right] \tag{89}$$

where N^σ_A and N^σ_B are the Sharvin conductances of the materials A and B forming the interface, in units of e^2/h .

The majority-spin case can be readily understood in terms of the geometry of the Fermi surfaces of Cu and Co so we begin by discussing this simple case before examining the more complex minority-spin channel.

Clean Cu|Co (111) Interface: Majority Spins

In the absence of disorder, crystal momentum parallel to the interface is conserved. If, for a given value of $\mathbf{k}_\parallel$, there is a propagating state in Cu incident on the interface but none in Co, then an electron in such a state is completely reflected at the interface. Conversely, $\mathbf{k}_\parallel$’s for which there is a propagating state in Co but none in Cu also cannot contribute to the conductance. To determine the existence of such states, it is sufficient to inspect projections of the Fermi surfaces of *fcc* Cu and majority-spin Co onto a plane perpendicular to the transport direction $\hat{n}$, shown in Fig. 16 for $\hat{n} = (111)$. The first feature to note in the figure (left-hand and middle panels) is that per $\mathbf{k}_\parallel$ there is only a single channel with positive group velocity so that the transmission matrix in (88) is a complex number whose modulus squared is a transmission probability with values between 0 and 1. It is plotted in the right-hand panel and can be interpreted simply. Regions which are depicted blue correspond to $\mathbf{k}_{\|}$'s for which there are propagating states in Cu but none in Co. These states have transmission probability 0 and are totally reflected. For values of $\mathbf{k}_{\|}$ for which there are propagating states in both Cu and Co, the transmission probability is very close to one, depicted red. These states are essentially free electron-like states which have the same symmetry in both materials and see the interface effectively as a very low potential step. Close to the center of the figure there is an annular region where there are propagating states in Co but none in Cu so they do not contribute to the conductance. Performing the sum in (88), we arrive at an interface conductance of $0.43 \times 10^{15}\ \Omega^{-1}\mathrm{m}^{-2}$ to be compared to the Sharvin conductances for Cu and Co of 0.56 and 0.47 respectively, in the same units for $a = 3.614\ \mathring{A}$ and an *spd* basis. The interface conductance of 0.43 is seen to be essentially the Sharvin conductance of the majority states of Co reduced because the states closest to the Λ-axis (corresponding to the symmetry axis of the figures, the ΓL line in reciprocal space) do not contribute.

Clean Cu|Co (111) Interface: Minority Spins

The minority-spin case is considerably more complex because the Co minority-spin d bands are only partly filled, resulting in multiple sheets of Fermi surface. These sheets are shown in Fig. 17 together with their projections onto a plane perpendicular to the (111) transport direction. Compared to Fig. 16, one difference we immediately notice is that even single Fermi surface (FS) sheets are not single valued: for a given $\mathbf{k}_{\|}$ there can be more than one mode with positive group velocity. The areas depicted green in the projections of the FS sheets from the fourth and fifth bands are examples where this occurs.

An electron incident on the interface from the Cu side, with transverse crystal momentum $\mathbf{k}_{\|}$, is transmitted into a linear combination of all propagating states with the same $\mathbf{k}_{\|}$ in Co; the transmission matrix $t^{\sigma}_{mn}(\mathbf{k}_{\|})$ is in general not square but rectangular. The transmission probabilities $T_{mn}(\mathbf{k}_{\|})$ are shown in the bottom row of Fig. 17. Because there is only a single incident state for all $\mathbf{k}_{\|}$, the maximum transmission probability is one. Comparison of the total minority-spin transmission probability $T_{\mathcal{LR}}(\mathbf{k}_{\|})$ (Fig. 17, bottom right-hand panel) with the corresponding majority-spin quantity (right-hand panel of Fig. 16) strikingly illustrates the spin-dependence of the interface scattering, much more so than the integrated quantities might have led us to expect; the interface conductances, 0.36 and $0.43 \times 10^{15}\Omega^{-1}\mathrm{m}^{-2}$ from Table 3.1.1, differ by only $\sim 20\%$.

Three factors contribute to the large $\mathbf{k}_{\|}$-dependence of the transmission probability: first and foremost, the complexity of the Fermi surface of both materials but especially of the minority spin of Co; secondly and inextricably linked with the first because of the relationship $\hbar v_{\mathbf{k}} = \nabla_k \varepsilon(\mathbf{k})$, the mismatch of the Fermi velocities of the states on either side of the interface. Thirdly, the orbital character of the states m and n which varies strongly over the Fermi surface and gives rise to large matrix element effects.

The great complexity of transition metal Fermi surfaces, clear from the figure and well-documented in standard textbooks, is not amenable to simple analytical treatment and has more often than not been neglected in theoretical transport studies. Nevertheless, as illustrated particularly well by the ballistic limit [77, 78], spin-dependent band structure effects have been shown to lead to magnetoresistance ratios comparable to what are observed experimentally in the current-perpendicular-to-plane (CPP) measuring configuration and cannot be simply ignored in any quantitative discussion. Most attempts to take into account contributions of the d states to electronic transport do so by mapping the five d bands onto a single tight-binding or free-electron band with a large effective mass.

Fermi surface topology alone cannot explain all aspects of the transmission coefficients seen in Fig. 17. For example, there are values of $\mathbf{k}_{\|}$, such as that labeled Y in the figure, for which propagating solutions exist on both sides of the interface yet the transmission probability is zero. This can be understood as follows. We begin by choosing a (1×1) interface unit cell so that the atoms which occupy the ABC sites

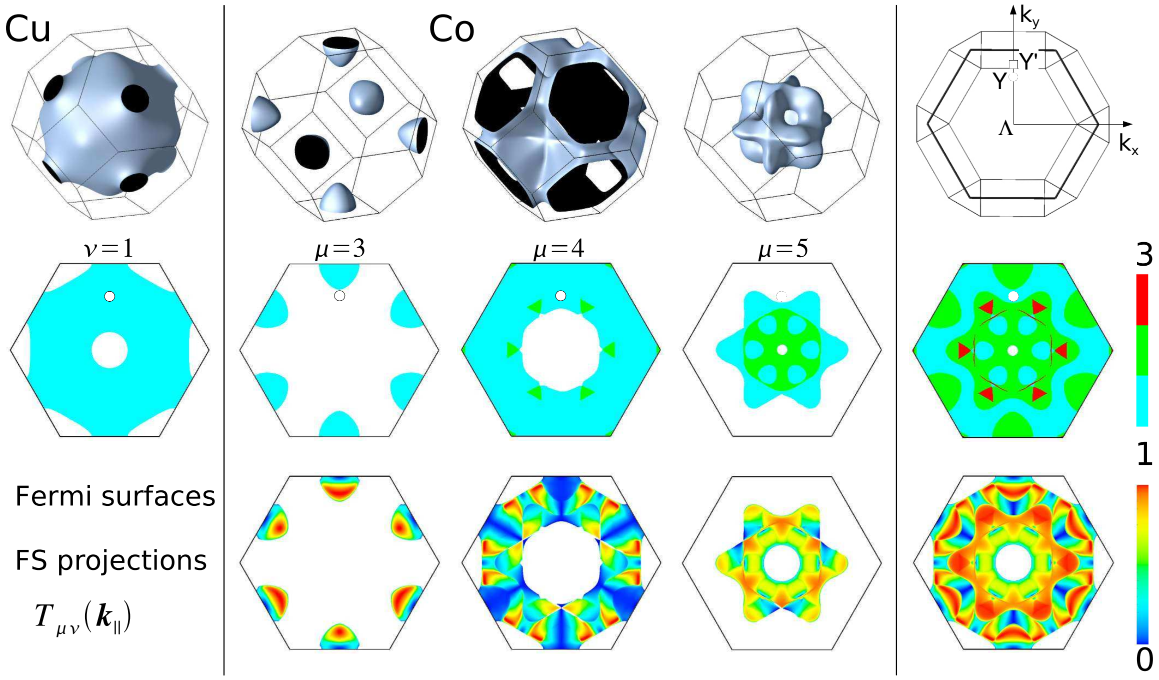

Figure 17: Top row, left-hand panel: Fermi surface (FS) of *fcc* Cu; middle panels: third, fourth and fifth FS sheets of minority-spin fcc Co; right-hand panel: projection of the bulk fcc Brillouin zone (BZ) onto a plane perpendicular to the (111) direction and of the two dimensional BZ. Middle row: corresponding projections of individual FS sheets and (rhs) of Co total. The number of propagating states with positive velocity is color-coded following the color bar on the right. Bottom row: probability $T_{\mu\nu}(\mathbf{k}_{\|})$ for a minority-spin state on the single FS sheet of Cu ($\nu = 1$) to be transmitted through a Cu|Co(111) interface into FS sheet μ of *fcc* Co as a function of the transverse crystal momentum $\mathbf{k}_{\|}$. The point Y (indicated by a small open circle) is such that there are only propagating states in Cu and in the fourth FS sheet of Co. For the point Y' (indicated by a small open square) which is slightly further away from Λ, there is, in addition, a propagating state in the third FS sheet of Co.

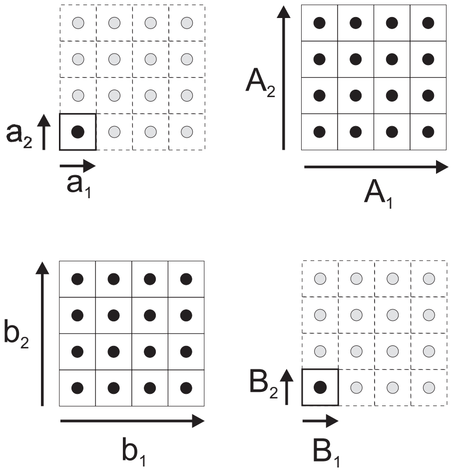

Figure 18: Illustration of lateral supercells and corresponding 2D interface Brillouin zones. Top panel: lattice vectors for a primitive unit cell containing a single atom (lhs) and a 4×4 supercell (rhs). Bottom panel: a single k-point in the BZ (rhs) corresponding to the 4×4 real-space supercell is equivalent to 4×4 k-points in the BZ (lhs) corresponding to the real-space primitive unit cell.

characteristic of the stacking in the *fcc* structure all lie along the y-axis. At $\mathbf{k}_{\|} = Y$, the propagating states in Cu have $\{s, p_y, p_z, d_{yz}, d_{3z^2-r^2}, d_{x^2-y^2}\}$ character and are even with respect to reflection in the plane formed by the y-axis and the transport direction perpendicular to the (111) plane which we choose to be the z-axis. For this $\mathbf{k}_{\|}$ the only propagating state in Co is in the fourth band. It has $\{p_x, d_{xy}, d_{xz}\}$ character which is odd with respect to reflection in the yz plane. Consequently, the corresponding hopping matrix elements in the Hamiltonian (and in the Green function) vanish and the transmission is zero.

Along the k_y axis the symmetry of the states in Cu and those in the fourth band of Co remain the same and the transmission is seen to vanish for all values of k_y. However, at points further away from Λ, we encounter states in the third band of Co which have even character whose matrix elements do not vanish by symmetry and we see substantial transmission probabilities. Similarly, for points closer to Λ, there are states in the fifth band of Co with even character whose matrix elements also do not vanish and again the transmission probability is substantial. Because it is obtained by superposition of transmission probabilities from Cu into the third, fourth and fifth sheets of the Co FS, the end result, though it may appear very complicated, can be straightforwardly analyzed in this manner k-point by k-point.

Though the underlying lattice symmetry is only threefold, the Fermi surface projections shown in Fig. 17 have six-fold rotational symmetry about the line Λ because bulk *fcc* structure has inversion symmetry (and time-reversal symmetry). The interface breaks the inversion symmetry so $T_{mn}(\mathbf{k}_{\|})$ has only threefold rotation symmetry for the individual FS sheets. However, in-plane inversion symmetry is recovered for the total transmission probability $T_{\mathcal{LR}}(-\mathbf{k}_{\|}) = T_{\mathcal{LR}}(\mathbf{k}_{\|})$ which has full sixfold symmetry.

3.2 Interface Disorder

Instructive though the study of perfect interfaces may be in gaining an understanding of the role electronic structure mismatch may play in determining giant magnetoresistive effects, all measurements are made on devices which contain disorder, in the diffusive regime. Because there is little information available from experiment about the nature of this disorder, it is very important to be able to model it in a flexible manner, introducing a minimum of free parameters. To model interfaces between materials with different lattice constants and disorder, we use *lateral supercells*.

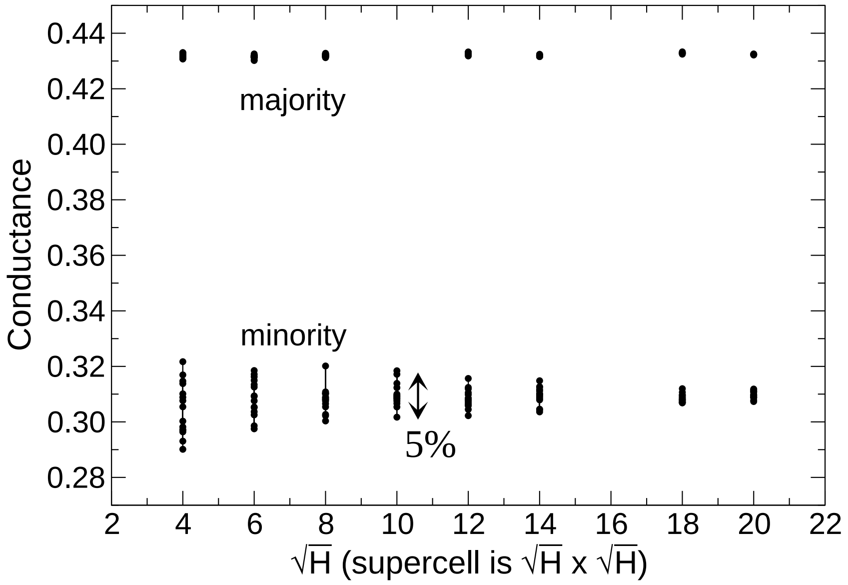

Figure 19: Interface conductance (in units of $10^{15}\Omega^{-1}\mathrm{m}^{-2}$) for a disordered Cu|Co (111) interface modeled as 2ML of 50%-50% alloy in a $\sqrt{H} \times \sqrt{H}$ lateral supercell as a function of $\sqrt{H}$. The results are given for different randomly generated configurations of disorder (15 for minority spin, 5 for majority spin). These results are for an *fcc* lattice constant of $a = 3.614\mathring{A}$, an *spd* basis and Perdew-Zunger exchange-correlation potential.

Lateral Supercells The TB-MTO scheme is computationally very efficient and allows us to use large lateral supercells to model in a simple fashion interface disorder, interfaces between materials whose underlying lattices are incommensurate, or quantum point contacts. This treatment becomes formally exact in the limit of infinitely large supercells. In practice, satisfactory convergence is achieved for supercells of quite moderate size.

The use of lateral supercells makes it possible to analyze diffuse scattering particularly simply. We consider an $H_1 \times H_2$ lateral supercell defined by the real-space lattice vectors

$$\mathbf{A}_1 = H_1\mathbf{a}_1 \quad \text{and} \quad \mathbf{A}_2 = H_2\mathbf{a}_2 \tag{90}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice vectors describing the in-plane periodicity of a primitive unit cell (Fig. 18). The cells contained within the supercell are generated by the set of translations

$$\left\{\mathbf{T}_{\|} = h_1\mathbf{a}_1 + h_2\mathbf{a}_2 \,;\, 0 \le h_1 < H_1,\, 0 \le h_2 < H_2\right\}. \tag{91}$$

In reciprocal space the supercell Brillouin zone is defined by the reduced vectors

$$\mathbf{B}_1 = \mathbf{b}_1/H_1 \quad \text{and} \quad \mathbf{B}_2 = \mathbf{b}_2/H_2 \tag{92}$$

where $\mathbf{b}_1$ and $\mathbf{b}_2$ are the reciprocal lattice vectors corresponding to the real space primitive unit cell. As a result the Brillouin zone (BZ) is folded down, as shown schematically in Fig. 18 (bottom rhs), and the single $\mathbf{k}_{\|}^{\mathbb{S}}$ point ($\mathbb{S}$ is used to label supercell quantities) in the supercell BZ corresponds to the set of $H_1 \times H_2$ $\mathbf{k}$ points in the original unfolded BZ

$$\left\{\mathbf{k}_{\|} = h_1\mathbf{B}_1 + h_2\mathbf{B}_2 \,;\, 0 \le h_1 < H_1,\, 0 \le h_2 < H_2\right\}. \tag{93}$$

Solutions associated with different $\mathbf{k}_{\|}$ in the primitive unit cell representation become different "bands" at the single $\mathbf{k}_{\|}^{\mathbb{S}}$ in the supercell representation.

The lead states are calculated using the translational symmetry of the primitive unit cell so that the computational effort scales linearly with the size of the supercell *i.e.* as $(H_1 \times H_2)$ rather than as $(H_1 \times H_2)^3$

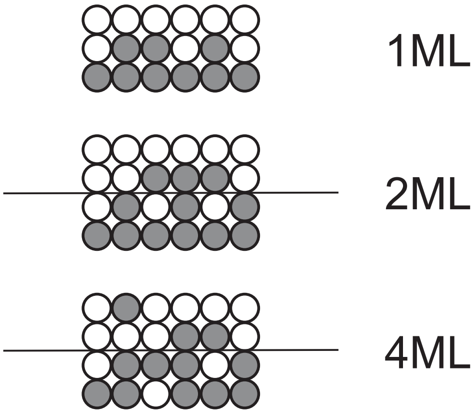

Figure 20: Illustration of 3 different models of interface disorder considered. Top (1ML): disorder is modeled using one monolayer (ML) of $[\mathrm{Cu}_{1-x}\mathrm{Co}_x]$ alloy between Cu and Co leads, denoted as $\mathrm{Cu}[\mathrm{Cu}_{1-x}\mathrm{Co}_x]\mathrm{Co}$. Middle (2ML): disorder modeled in two MLs as $\mathrm{Cu}[\mathrm{Cu}_{1-x}\mathrm{Co}_x|\mathrm{Cu}_x\mathrm{Co}_{1-x}]\mathrm{Co}$. Bottom (4ML): starting from the 2 ML disorder case, 1/3 of the concentration x of impurity atoms is transferred to the next layer resulting in disorder in four MLs: $\mathrm{Cu}[\mathrm{Cu}_{1-\frac{x}{3}}\mathrm{Co}_{\frac{x}{3}}|\mathrm{Cu}_{1-\frac{2x}{3}}\mathrm{Co}_{\frac{2x}{3}}|\mathrm{Cu}_{\frac{2x}{3}}\mathrm{Co}_{1-\frac{2x}{3}}|\mathrm{Cu}_{\frac{x}{3}}\mathrm{Co}_{1-\frac{x}{3}}]\mathrm{Co}$.

which is the scaling typical for matrix operations. Another advantage is that it enables us to analyze the scattering. By keeping track of the relation between supercell "bands" and equivalent eigenmodes at different $\mathbf{k}_\parallel$ (Fig. 18) we can straightforwardly obtain $t_{mn}(\mathbf{k}_{\parallel 1}, \mathbf{k}_{\parallel 2})$ and other scattering coefficients. In other words the "interband" specular scattering in the supercell picture translates, in the presence of disorder in the scattering region, into the "diffuse" scattering between the $\mathbf{k}_\parallel$ vectors belonging to the set (93). Since this approach is formally only valid if sufficiently large supercells are used, we begin by studying how the interface conductance depends on the lateral supercell size.

To perform fully self-consistent calculations for a number of large lateral supercells and for different configurations of disorder would be prohibitively expensive. Fortunately, the coherent potential approximation (CPA) is a very efficient way of calculating charge and spin densities for a substitutional disordered A_xB_{1-x} alloy with an expense comparable to that required for an ordered system with a minimal unit cell [79]. The output from such a calculation are atomic sphere potentials for the two sites, υ_A and υ_B. The layer CPA approximation generalizes this to allow the concentration to vary from one layer to the next [66].

Once υ_A and υ_B have been calculated for some concentration x, an $N \times N$ lateral supercell is constructed in which the potentials are distributed at random, maintaining the concentration for which they were calculated self-consistently. For a given value of N, a number of such random distributions is generated. The conductances calculated for $4 \leq N \leq 20$ are shown in Fig. 19 for a Cu|Co(111) interface in which the Cu and the Co layers forming the interface are totally mixed to give two layers of 50%-50% interface alloy. The sample-to-sample variation is largest for the minority spin case, ranging from ±5% for a modest 4×4 unit cell and decreasing to about ±0.5% for a 20×20 unit cell. For $N \sim 10$, the spread in minority spin conductances is $\sim 3\%$ which is comparable to the typical uncertainty we associated with the LDA error, the uncertainty in lattice constants or the error incurred by using the ASA.

Comparing the conductances without and with disorder, we see that disorder has virtually no effect on the majority spin channel (0.43 versus $0.43 \times 10^{15}\,\Omega^{-1}\mathrm{m}^{-2}$) which is a consequence of the great similarity of the Cu and Co majority spin potentials and electronic structures. However, in the minority-spin channel the effect (0.36 versus $0.31 \times 10^{15}\,\Omega^{-1}\mathrm{m}^{-2}$) is much larger. Equation (89) can be used to obtain estimates

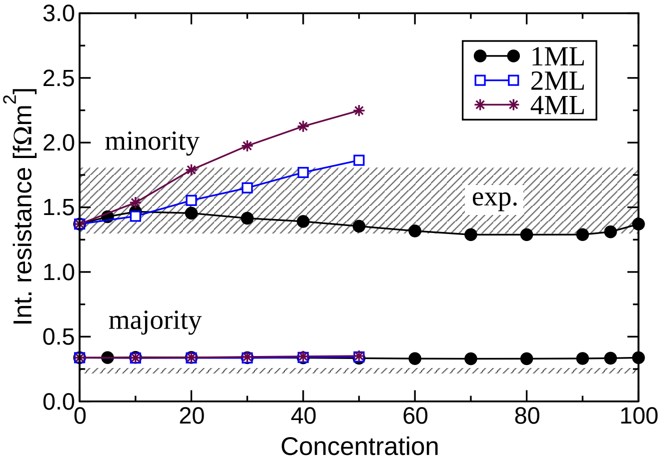

Figure 21: Interface resistance for disordered interfaces as a function of the alloy concentration used to model disordered interfaces calculated using (89). The experimental values for sputtered and MBE grown multilayers cited in Table I of Ref. [69] span a range of values which is indicated by the shaded regions.

of the interface resistances R_σ^{Schep}, which can be compared to values extracted from experiment [69, 80]. Theoretical values derived in this way for the different models of interface disorder shown in Fig. 20 are compared with experiment in Fig. 21.

The agreement of the computed interface resistances with experiments, which was already found to be good for specular interfaces of the Cu|Co systems [3, 68], is improved for minority spins by including interface disorder [7]. However, for the majority-spin case, the calculated interface resistance is *larger* than the value extracted from experiment, whether or not interface disorder is included. We will return to this again briefly after discussing how the interface scattering can be analyzed.

3.2.1 Analysis of Interface Disorder Scattering: Cu|Co

When disorder is modeled using lateral supercells, the transmission matrix elements can be categorized as being either *ballistic* or *diffuse*, depending upon whether or not transverse momentum is conserved. The scattering induced by two layers of 50%-50% alloy is illustrated in Figs. 22 and 23 for the majority and minority spins, respectively, of a Cu|Co(111) interface. The calculations were performed for a single $\mathbf{k}_\parallel$ point, Γ, and a 20×20 lateral supercell, equivalent to using a 1×1 interface cell and k-space sampling with 20×20 points in the corresponding BZ. Figs. 22(a) and 22(b) show the majority-spin Fermi surface projections of *fcc* Cu and Co, respectively, and the coarse 20×20 grid is seen to yield a good representation of the detailed Fermi surface projections shown in Fig. 16. The probability, $T(\mathbf{k}_\parallel, \mathbf{k}'_\parallel)$, that a state in Cu with transverse momentum $\mathbf{k}_\parallel$ is scattered on transmission through the disordered interface into the state in Co with transverse momentum $\mathbf{k}'_\parallel$, is shown in Fig. 22(c) for $\mathbf{k}_\parallel = Y$ on the k_y axis (see the inset in Fig. 17) and is dominated by the $\mathbf{k}_\parallel$-conserving forward scattering, the *specular transmission*: $T(\mathbf{k}_\parallel = Y, \mathbf{k}_\parallel = Y) = 0.93$. Indeed, the diffuse scattering is so weak that it cannot be seen on a scale of T from 0 to 1. To render it visible, a magnification by a factor 500 is needed, shown in Fig. 22(d). The total diffuse scattering, $T_{diff}(Y) = \sum_{k'_\parallel \neq k_\parallel} T(\mathbf{k}_\parallel = Y, \mathbf{k}_\parallel \neq Y) = 0.04$ can be seen from the figure to be made up of contributions of $T \sim 0.0004$ per $\mathbf{k}_\parallel$-point from roughly a quarter of the BZ (100 $\mathbf{k}_\parallel$ points) centered on $\mathbf{k}_\parallel = Y$. The total transmission, $T_{total} = T_{spec} + T_{diff} = 0.93 + 0.04 = 0.97$, compared to a transmission of 0.99 in the absence of disorder. In the majority case, there is thus a strong specular transmission peak surrounded by a weak diffuse background.

The minority-spin Fermi surface projections of *fcc* Cu and Co are shown in Figs. 23(a) and 23(b),

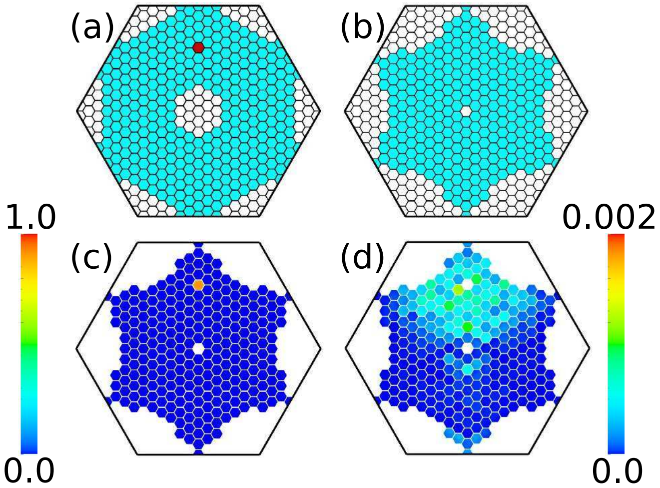

Figure 22: Fermi surface projections of majority-spin *fcc* Cu (a) and Co (b) derived from a single k-point using a 20×20 lateral supercell. The dark red point in the Cu Fermi surface projection corresponds to the point Y in the top right-hand panel of Fig. 17. $T(Y, \mathbf{k}'_{\|})$ is shown in (c), and in (d) magnified by a factor 500 where the ballistic component $T(Y, \mathbf{k}'_{\|} = Y)$ is indicated by a white point because its value goes off the scale. The results were obtained by averaging over 5 different configurations of disorder.

respectively. Compared to the corresponding panels in Fig. 17, the 20×20 point representation is seen to be sufficient to resolve the individual Fermi surface sheets of Co. To study the effect of scattering, we consider two different situations. In the first, we again consider $\mathbf{k}_{\|} = Y$, for which the transmission in the absence of disorder was zero as a result of the symmetry of the states along the k_y axis. $T(\mathbf{k}_{\|} = Y, \mathbf{k}_{\|})$ is shown in Fig. 23(c). By contrast with the majority-spin case just examined, there is now scattering to all other k-points in the 2D BZ, $\sum_{k'_{\|} \neq k_{\|}} T(\mathbf{k}_{\|} = Y, \mathbf{k}_{\|} \neq Y) = 0.58$. The specular transmission $T(Y, Y)$ has increased from 0.00 in the clean case, to only 0.01 in the presence of disorder. The effect of disorder is to increase the total transmission, $T_{total}(Y) = \sum_{k'_{\|}} T(\mathbf{k}_{\|} = Y, \mathbf{k}_{\|})$ from 0.00 to $T_{spec}(Y) + T_{diff}(Y) = 0.01 + 0.58 = 0.59$. Disorder thus *increases* the transmission for states which were strongly reflected in its absence.

The second case we consider is that of a k-point slightly further away from the origin Λ along the k_y axis which had a high transmission, $T(Y') = 0.98$, in the absence of disorder. For this k-point, $T(\mathbf{k}_{\|} = Y', \mathbf{k}_{\|})$, shown in Fig. 23(d), looks very similar to Fig. 23(c). There is strong diffuse scattering with $\sum_{k'_{\|} \neq k_{\|}} T(\mathbf{k}_{\|} = Y', \mathbf{k}_{\|} \neq Y') = 0.54$ while $T(Y', Y')$ has been drastically decreased from 0.98 in the clean case, to 0.06 as a result of disorder. The total transmission, $T_{total}(Y') = T_{spec}(Y') + T_{diff}(Y') = 0.06 + 0.54 = 0.60$, is almost identical to what was found for the Y point. The effect of disorder has been to *decrease* the transmission of states which, in its absence, were weakly reflected. The strong k-dependence of the transmission found for the minority-spin channel in the specular case is largely destroyed by a small amount of disorder.

To derive (89), it was assumed that there is loss of coherence between adjacent interfaces. The scattering of majority-spin electrons at the Cu|Co(111) interface is so weak that this assumption is not obviously valid. It can be examined by seeing whether or not the total resistance of a Cu|Co multilayer containing N interfaces scales linearly with N. If this is so, then the incremental interface resistance $R(N) - R(N-1)$ should be independent of N. Note that the lead correction in (89) is independent of N and thus drops out of the incremental resistance.

The results of an extensive series of calculations for a disordered $\mathrm{Cu}_{10}|\mathrm{Co}_{10}(111)$ multilayer attached

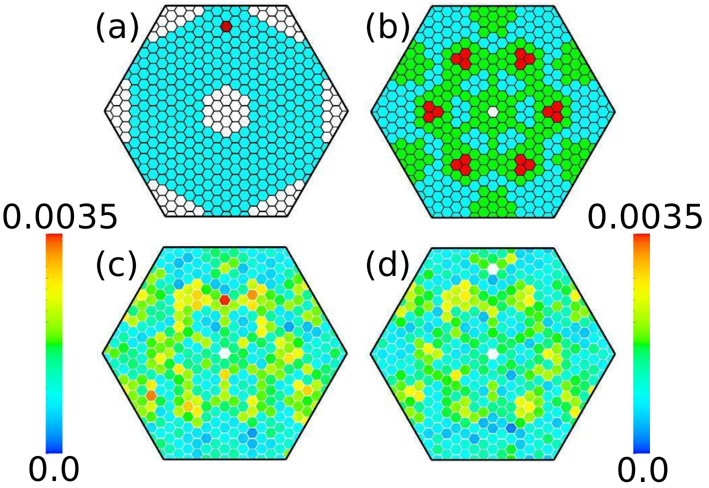

Figure 23: Fermi surface projections of minority-spin *fcc* Cu (a) and Co (b) derived from a single k-point using a 20×20 lateral supercell. The dark red point in the Cu Fermi surface projection corresponds to the point Y' in the top right-hand panel of Fig. 17. (c) $T(Y, \mathbf{k}'_{||})$ and (d) $T(Y', \mathbf{k}'_{||})$ calculated using 20 different disorder configurations; the ballistic component $T(Y', \mathbf{k}'_{||} = Y')$ is indicated by a white point because its value goes off scale. The results were obtained by averaging over 20 different configurations of disorder.

to Cu leads are shown in Fig. 24 which includes experimental values [69] for comparison. An 10×10 lateral supercell was used so that, according to Fig. 19, the error on the interface transmission due to configuration averaging is negligible for the majority-spin case and of order 5% for the minority spins. In the largest calculation represented in Fig. 24, the scattering region contained about 15000 atoms: 10 × 10 lateral supercell × 150 principal layers. For the strongly scattered minority spins, the interface resistance is essentially constant for all N (within the error bar of the calculation set by the configuration averaging, choice of exchange-correlation potential etc.). For the majority spin case there is a sharp drop before the incremental resistance levels off to a constant value for $N \geq 4$ which is a factor 3 4 lower than the experimental value. This implies a breakdown of the series resistor model for the majority spins or else there is some other source of majority-spin scattering which has not been included in the calculation. Including bulk scattering does not change this result significantly. Other materials specific studies of the transport properties of Cu|Co multilayers carried out with other methods [81] also find that substitutional disorder alone cannot account for the reported resistivities in the majority-spin channel.

3.2.2 Cr|Fe (100)

An extreme example of how interface disorder can *enhance* interface transmission is found for the bcc(100) orientation of Cr|Fe. Whereas the majority-spin band structures were well matched in the case of Cu|Co, the situation is reversed for Cr|Fe and it is the minority-spin electronic structures which match well. Calculating the interface resistance SR using (89), we find values of 3.73 fΩm^2 and 0.49 fΩm^2 for majority and minority spin, respectively, in the absence of disorder and values of 1.27 fΩm^2 and 0.47 fΩm^2, respectively when interface disorder is modeled as two layers of 50-50 alloy as was done for Cu|Co. Thus disorder reduces the majority-spin interface resistance by almost a factor of three while having only a small effect on the well-matched minority spin channel, just as in the Cu|Co majority spin case.

The qualitative difference between Cr|Fe and Cu|Co can be understood in terms of their Fermi surface

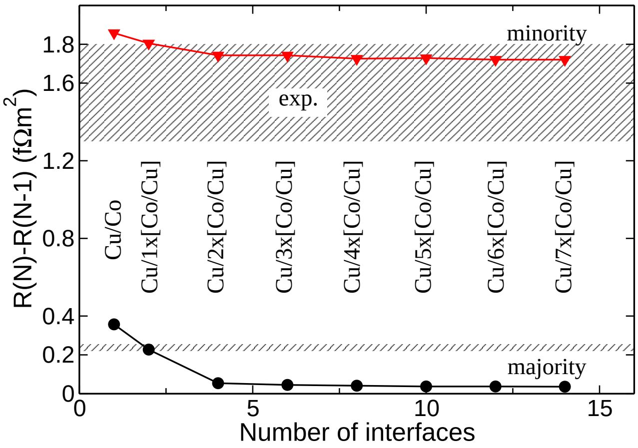

Figure 24: Differential interface resistance as the number of interfaces increase for a disordered Cu|Co(111) multilayer embedded between Cu leads. A 10 × 10 lateral supercell was used and the interface was modeled as two layers of 50%-50% alloy (2ML model). The results represent an average over 5 disorder configurations. The range of experimental values [69] is indicated by the shaded regions.

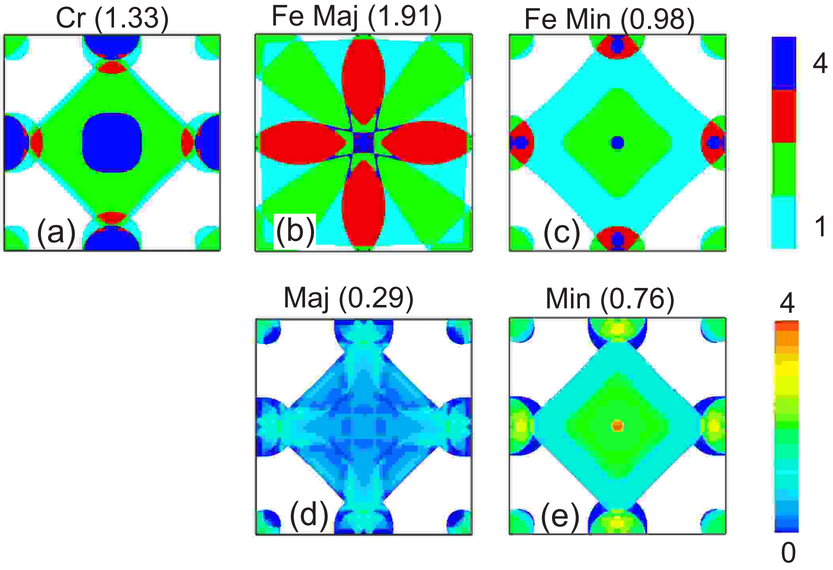

Figure 25: Fermi surface projections of *bcc* (a) non-magnetic Cr, (b) Fe, majority-spin and (c) Fe, minority-spin. (d) and (e) show the majority- respectively, minority-spin interface transmissions for a clean lattice-matched *bcc* Cr|Fe interface. The result of integrating the number of channels over the whole Brillouin zone is given in brackets at the top of each panel.

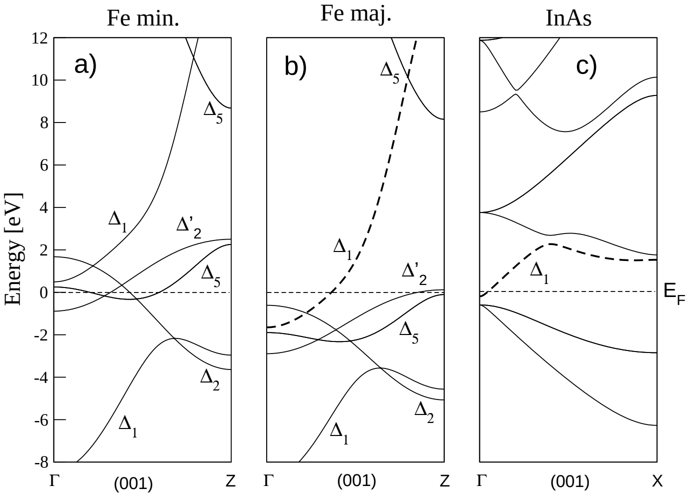

Figure 26: Energy band structures of tetragonal Fe minority spin states (a), majority spin states (b), and InAs states (c) at $\mathbf{k}_{\parallel} = 0$ for $\mathbf{k} = (00k_z)$ perpendicular to the interface.

projections and transmission probabilities $T_{\mathcal{LR}}(\mathbf{k}_{\parallel})$. In the Cu|Co(111) majority-spin case (Fig. 16), there was a large area of the 2D BZ where states on both sides matched very well and interface disorder led to mainly forward scattering with virtually no reduction of the total transmission. In the minority-spin case (Fig. 17), the situation was more complicated because the average transmission was much lower in the absence of disorder (∼ 60%) and the disorder-induced reduction of the interface transmission (∼ 20%) resulted from two competing effects: transmission enhancement by symmetry-breaking for channels which were closed for reasons of symmetry and transmission reduction by diffuse scattering for channels which were very transparent in the absence of disorder. On balance, defect scattering reduced the transmission probability and thus *increased* the interface resistance of the Cu|Co minority spin channel.

In spite of there being multiple sheets of Cr and majority-spin Fe Fermi surfaces which overlap in large regions of the 2D Brillouin zone (see Figs. 25(a-c)), the average majority-spin transmission probabilities in the absence of disorder, shown in Fig. 25(d), are very small throughout the BZ while those for the minority-spin case, shown in Fig. 25(e), are quite substantial. As in the Cu|Co case, there are two mechanisms by which interface disorder *increases* the interface transmission. Majority-spin electrons with small $\mathbf{k}_{\parallel}$ are almost completely reflected at the clean Cr|Fe interface because the electronic states on both sides of the interface do not match well. Defect scattering is found to increase the transmission of these electrons strongly. Furthermore, for large areas of the two-dimensional Brillouin zone, there are no propagating states on the Cr side. Propagating modes in Fe with these values of $\mathbf{k}_{\parallel}$, which were inaccessible to Cr electrons in the ordered case, can be reached by diffusive scattering. This opens up a large number of new channels and this increase in transmission for the Cr|Fe majority-spin channel translates into a reduction by a factor 3 of the interface resistance. Recent CPP experiments on Fe|Cr(110) [82] show that the spin-averaged resistance agrees very well with the theoretical prediction, but not the polarization dependence.

3.2.3 Spin-injection, spin-tunneling

Spin-dependent matching of electronic structures not only plays a role at interfaces between metallic ferromagnets and non-magnetic metals. It also occurs at the interface between itinerant ferromagnets and semiconductors or insulators[14] where the electronic structure of the semiconductor/insulator in a very

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[14] The term "Spintronics" is used to refer to the study of spin-dependent transport in semiconductors while "Magnetoelectronics" is used to refer either to spin-dependent transport in metallic systems or to spin-dependent

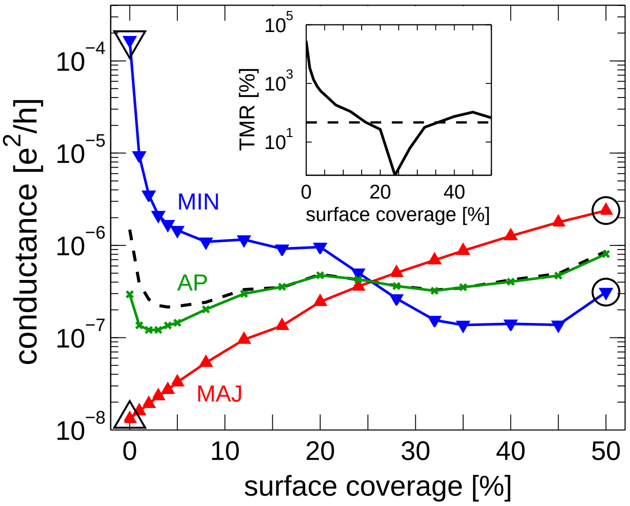

Figure 27: Configuration-averaged conductances G_P^{min} (▼), G_P^{maj} (▲), and G_{AP}^{σ} (×) of an Fe|vacuum|Fe magnetic tunnel junction with 8 ML thick vacuum barrier as a function of the surface coverage, normalized to a 1 × 1 surface unit cell. The dashed line denotes $G_{AP}^{\sigma} = \sqrt{G_P^{maj} G_P^{min}}$. Inset: TMR as a function of the surface coverage. The dashed line is the value predicted using Julliere's expression and a calculated DOS polarization of 55%.

small region of reciprocal space dominates the injection/tunneling as in Fig. 26. This happens when there is lattice matching and in the absence of disorder so transverse crystal momentum is conserved. Most work has focussed on systems containing Fe(001)-related interfaces because in this orientation the lattice constant of Fe is reasonably well matched to those of a number of inorganic semiconductors and to MgO. The electronic structures were either calculated directly from first-principles [20, 39, 83–91] or obtained by fitting to first-principles electronic structures [16, 18, 21, 22, 92]. For disorder-free interfaces, very large polarizabilities of the injection or tunnel currents are predicted, much larger than those measured so far, including the recent experiments on single-crystal MgO-based tunnel junctions [93–95].

Unlike metallic systems, the current in semiconductors or tunnel junctions is carried by a very small number of channels. A realistic description of transport in such systems requires describing these channels accurately. Calculations in which interface roughness and/or disorder were considered [39, 42] show that injection polarization depends sensitively on the detailed interface structure. Even a small amount of roughness (Fig. 27) or disorder (Fig. 28) is sufficient to quench the huge theoretical values of tunneling magnetoresistance predicted for ideal magnetic tunnel junctions to values comparable to those observed in experiment. While the quality of tunnel junctions is clearly improving, much more work needs to be done to characterize the experimental disorder quantitatively.

3.3 Outlook

So far we have been concerned with the quantitative and qualitative characteristics of the transmission and reflection of electron states at *single* interfaces between real materials, one of which is an itinerant ferromagnet. The advantage of focussing on the full scattering matrix, rather than simply calculating the conductance, is that it provides us with greater insight and is a very convenient point of contact with other theories, such as random matrix theory [30] or circuit theory [31]. By interfacing with phenomenological theories, we can make contact relatively easily with more complex transport problems. A

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transport in general, including both Spintronics, giant magnetoresistance (GMR) and tunneling magnetoresistance (TMR).

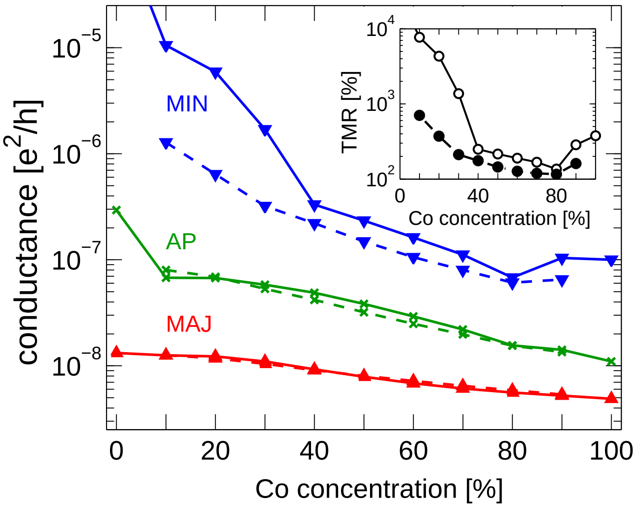

Figure 28: G_P^{min} (▼), G_P^{maj} (▲), and G_{AP}^{σ} (×) for an $\mathrm{Fe}_{1-x}\mathrm{Co}_x$|vacuum|$\mathrm{Fe}_{1-x}\mathrm{Co}_x$ magnetic tunnel junction with 8 ML thick vacuum barrier as a function of x, the concentration of Co atoms, calculated in the virtual crystal (VCA: solid lines) and CPA/supercell (SC: dashed lines) approximations. Conductances are configuration averaged and normalized to a 1×1 surface unit cell. Inset: TMR in VCA (○) and CPA/SC (●) approximations.

good example of this is the study of the materials dependence of the suppression of Andreev scattering at a ferromagnetic|superconducting interface. This is a problem which had been studied phenomenologically [30] without taking into account details of the electronic structure of materials which might be used in an actual experiment. Because it had been formulated in terms of the scattering matrix for the F|S interface with the superconducting material in its normal state, it was straightforward to introduce and study the dependence on the constituent materials [38]. We argue that such an approach may be more fruitful than a frontal, brute force approach to calculating transport properties entirely from first principles.

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