Ψ_k Newsletter

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

Number 55 February 2003

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Contents

1 Editorial

In this newsletter we would like to turn readers' attention to the **General News Section** where we correct some incorrect statements on the FP6 RT networks, made in the report on the Midterm and Annual Meeting of the RTN1 published in the December issue. Then in the following section, **News from the RTN1** we have two reports, of which one is on recent *Conference on Nanoelectronics*, that took place in Lancaster early January. This report contains abstracts of presented papers. In the same section there are announcements of forthcoming workshops on "Spin Mesoscopics" and "Diluted Magnetic Semiconductors", and a summer school on "New Magnetics". In the section of the new RTN on "f-electrons" (**RTN2**) we have one postdoctoral position announcement. The other position announcements can be found in the usual section **General Job Announcements**. In the section **News from the ESF Programme** we have three contributions by Professor Volker Heine, the chairman of this Psi-k ESF Programme. The first of them is the report on the 2002 activities within the programme, the second brings some latest news on the new Psi-k ESF Programme, and the last is about a completely new initiative for our whole community associated with the I3 initiative of EU. In the same section we have minutes of the Steering Group of the Psi-k ESF Programme. Finishing the section are three announcements of forthcoming meetings organized with the financial support of the Psi-k ESF Programme. In the **News from UK's CCP9 Programme** section there is a second announcement of a conference in Bristol that is to be *a celebration of the contributions of Balazs Győrffy to theories of the electronic structure of solids.* The title of the conference is *"Order and disorder in solids: alloys, magnetism and superconductivity"*, and it will take place on April 11-12, 2003. In the **General Workshop/ Conference Announcements** section we announce the *Nineth Wien Workshop.* Abstracts of newly submitted papers are in the following section. Then comes a section on **Presenting Other Initiatives** where readers will find some information on upgrade of *CPMD code*, and *free software project for atomistic-scale computation.* The newsletter is finished with the **Scientific Highlight of the Month** section, and the highlight is by Heike Herper (*Duisburg* and *Vienna*), the RTN1 postdoctoral fellow of Vienna's node, and the title is **"Electric transport perpendicular to the planes"**. Please check tables of contents for further details on this newsletter.

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 some of the Psi-k 2003 workshops and hands-on courses (subject to funding). In these pages you can also find information on how to apply for funding to make collaborative visits.

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@daresbury.ac.uk	**messages to the coordinators, editor & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB of all Networks**
psik-network@daresbury.ac.uk	**messages to the whole Ψ_k community**

Dzidka Szotek and Walter Temmerman
e-mail: psik-coord@dl.ac.uk

2 General News

2.1 Correction to the 6th Framework Programme (FP6) RT Networks

In the previous Psi-k Newsletter (issue 54), in the report on the RTN1 Midterm Review and Annual Meeting, it was incorrectly stated that "... the EU will not continue with these type of Training Networks ...", meaning the Research and Training Networks (RTNs).

It has been pointed out by Raymond Monk, the EU project officer for the physics RTNs, that **" ... Research Training Networks will, in fact, continue during the new programme and will have a boost in funding compared to FP5. There will be some changes regarding the increased involvement of researchers outside Europe and the removal of the age limit but the basic recipe will remain the same including the support for research in any area (including basic research) ..."**.

The new WebPages for all the FP6 researcher mobility and training "Marie Curie" actions are as follows:

http://europa.eu.int/mariecurie-actions/

and Raymond Monk would recommend that the following document be downloaded from this website (also found in the "publications" section)

`http://europa.eu.int/comm/research/fp6/mariecurie-actions/pdf/mcguide_en.pdf` .

We apologize for the misunderstanding and encourage all interested to consult the above Web-Pages.

Z. (Dzidka) Szotek

3 News from the RTN1

COMPUTATIONAL MAGNETOELECTRONICS

3.1 Reports on RTN1 Workshops

3.1.1 Report on the International Conference on Nanoelectronics

International Conference on Nanoelectronics

Lancaster, 4-9 January 2003

Sponsored by
European Science Foundation - STRUC Ψ_k Programme
RTN on "Computational Magnetoelectronics"
CCP9
EPSRC
Institute of Physics (Semiconductor Physics Group)
NWDA Science
Lancaster University

Organized by
V.I. Fal'ko (Lancaster), C.J. Lambert (Lancaster),
and W. Temmerman (Daresbury)

The conference brought together more than 200 researchers actively working in the rapidly developing areas of nanoelectronics, interface physics and nanostructured materials. 22 topical oral sessions and 86 presentations during the Poster session encompassed physics of nanoelectronic devices and materials interfaces; quantum transport and noise; spin-dependent transport and control; mesoscopic superconductors; proximity effects and hybrid structures; molecular-scale electronics and atomic contacts; ab initio modelling of materials and interfaces; correlation effects in quantum dots (including Kondo effect), phase coherence effects in wires and rings. Special attention has been paid to the material science aspects of quantum manipulation and the physics of various solid state prototypes of qubits. More than 50 invited speakers represented internationally leading groups working at the forefront of research in all these areas of solid state physics. Those included: C Beenakker (Leiden), F Beltram (Pisa), P Beton (Nottingham), S Blügel (Julich), A Brataas (Trondeim), M Büttiker (Geneva), B Bulka (Poznan),

V Chandrasekhar (Northwestern U), P Delsing (Chalmers), A Geim (Manchester), K Ensslin (ETH Zurich), R Fazio (Pisa), A Fert (Orsay), M Finnis (Belfast), B Gallagher (Nottingham), L Glazman (Minneapolis), P Hakonen (LTL Espoo), R Haug (Hannover), D Haviland (Stockholm), F Hekking (Grenoble), T Jungwirth (Prague), P Kelly (Twente), J Kotthaus (Munich), M Krawiec (Bristol), L Lévy (Grenoble), I Lerner (Birmingham), P Lindelof (Copenhagen), D Loss (Basel), A MacDonald (Austin), D Mailly (Marcoussis), C Marcus (Harvard), L Molenkamp (Würzburg), H Mooij (Delft), Y Nazarov (Delft), B Pannetier (Grenoble), F Peeters (Antwerp), V Petrashov (Royal Holloway), J-L Pichard (Saclay), J von Ruitenbeek (Leiden), C Schönenberger (Basel), R Shekhter (Chalmers), A Shields (Toshiba Cambridge), M Skolnick (Sheffield), U Sivan (Technion), F Sols (Madrid), K Stokbro (TU- Lyngby), T Schulthess (Oakridge NL), H Takayanagi (NTT Atsugi), D Tomanek (Michigan), C Urbina (Saclay), L Vandersypen (Delft), B van Wees (Groningen), J Weis (MPI-Stuttgart), D Williams (Hitachi Cambridge), A Yacoby (Weizmann Inst.), N Zhitenev (Lucent - Bell Labs).

Vladimir I Fal'ko and Edward McCann

Programme

Saturday 4th	
Conference opening	
M: Materials and interfaces I	
Chair: Walter Temmerman	
Mike Finnis	Ab initio calculations at interfaces
Stefan Blügel	Interface Magnetism at the age of spintronics
Dzidka Szotek	Half-metallic transition metal oxides
F: Diluted Magnetic Semiconductors (DMS)	
Chair: Vladimir Falko	
Tomas Jungwirth	Transport properties of diluted magnetic semiconductor ferromagnets
Thomas Schulthess	The electronic state of Mn impurities in III-V semiconductors
Francois Peeters	Manipulation of spin in DMS

Sunday, 5th	
S: Mesoscopic superconductors	
Chair: Colin Lambert	
Pertii Hakonen	Oscillating Josephson junction
James Annett	Theory of half-integer flux quantization in d-wave superconducting rings
Robert Shekhter	Shuttling of single electrons and Cooper pairs
David Haviland	Cooper pair tunnelling and Coulomb blockade
M: Magneto-transport and spin	
Chair: Tomas Jungwirth	
Paul Kelly	Materials-specific theory for spin electronics
Bryan Gallagher	Magneto-transport in high quality GaMnAs
Edward McCann	Magnon-assisted transport in ferromagnetic junctions
M: Nano-electronic materials: Optics	
Chair: Philip Buckle	
Maurice Skolnick	Optics of single self-assembled quantum dots
Thierry Martin	Noise correlation and Bell inequalities
Andrew Shields	Single photon generation and detection using semiconductor quantum dots
M: Molecular electronics I	
Chair: Nicolas Agrait	
Nikolai Zhitenev	Conductance of gated metal-molecule-metal nano-junctions
Kurt Stokbro	Transiesta: A spice for molecular electronics
Georgios Fagas	Conductance of a molecular junction mediated by electrode surface states
Uri Sivan	Molecular shift registers
D: Correlations and Kondo effect in dots	
Chair: Igor Lerner	
Bogdan Bulka	Coherent transport and electronic correlations in magnetic nano-devices
Jan von Delft	SU(4) Fermi liquid state in a double quantum dot system
Jurgen Weis	Kondo effect in single and electrostatically coupled quantum dot systems
Jurgen König	Aharonov-Bohm interferometry with interacting quantum dots

M: Molecular electronics II

Chair: Kurt Stokbro

Peter Beton	Assembly and processing of organic nanostructures
Rosa Di Felice	Theoretical modelling of DNA-based nanowires
David Tomanek	Nanoelectronics with carbon
Gunther Lientschnig	Electrical measurements on phenylene-based conjugated molecules

D: Transport in quantum dots

Chair: Klaus von Klitzing

Charles Marcus	Spin and symmetry in mesoscopic conductance and rectification
Rolf Haug	Transport through quantum rings and dots
Vincent Bayot	Quantum transport in ballistic cavities subject to a strictly parallel magnetic field
John Jefferson	Two-electron quantum dots and scalable Qubits

Monday 6th

T: Correlations and quantum transport

Chair: Yuli Nazarov

Leonid Glazman	Transport anomalies in multi-mode Luttinger liquids
Igor Lerner	Zero-bias anomaly in the absence of equilibrium
Stefan Kettemann	Kondo enhanced Anderson localisation
Rodolfo Jalabert	Transport through strongly correlated systems

M: Materials and interfaces II

Chair: Stefan Blügel

Fabrizio Cleri	Modelling the electrical conductivity at grain boundaries and surfaces
Ingrid Mertig	Stability and transport in nano-contacts: An ab initio description
Mariusz Krawiec	FFLO state in FM/SC heterostructures
Allan MacDonald	Interplay of collective and quasi-particle degrees of freedom in DMS and metallic ferromagnets

S: Mesoscopic superconductors and hybrid structures I

Chair: Venkat Chandrasekhar

Hideaki Takayanagi	Ferromagnetism and superconductivity in artificial crystals
Mattias Eschrig	Theory of half metal - superconductor heterostructures
Gilles Montambaux	Mesoscopic NS rings: From persistent to Josephson current

T: Quantum transport and noise	
Chair: Christian Glattli	
Denis Basko	Dynamic localization in quantum dots: Analytical theory
Alex Savchenko	Shot noise in transport via localised states
Yuli Nazarov	Interactions, resonant tunnelling and transmission distribution
M: Atomic-size contacts and molecular electronics	
Chair: Uri Sivan	
Jan van Ruitenbeek	Atomic-size conductors: Chains of atoms and hydrogen molecules
Matthias Hettler	Transport through molecules
Nicolas Agrait	Forces and vibration modes in a chain of single gold atoms
Poul Lindelof	Electron spin in carbon nanotubes
Sophie Gueron	Superconductivity of carbon nanotubes
Andrew Briggs	Quantum computing with nanoelectronics structures
Tuesday 7th	
S: Decoherence and noise in metals and superconductors	
Chair: Per Delsing	
Wolfgang Belzig	Phase-sensitive shot noise in an Andreev interferometer
Marcus Büttiker	Chaotic dot - superconductor analogy of the Hanburry Brown Twiss effect
Laurent Lévy	Spectroscopy and decoherence in double-island Qubits
Carlo Beenakker	Pascal distribution of voltage fluctuations out of equilibrium
T: Quantum transport and correlations	
Chair: Mark Sanquer	
Amir Yacoby	Imaging localization in the quantum Hall regime
Rolf Crook	Scanned gate microscopy to investigate transport in disordered 1D wires
Roberto Raimondi	Non-linear transport and quantum interaction corrections in disordered systems
Jean-Louis Pichard	Electron super-solid on square lattices
D: Quantum dots and Qubits	
Chair: Charles Marcus	
Jörg Kotthaus	Coherent transport and electronic interactions in quantum dots
Klaus Ensslin	Spin effects in quantum dots and quantum rings
Christopher Ford	Kondo effect in an anti-dot in the quantum Hall regime
David Williams	Semiconductor structures for quantum information processing
Daniel Loss	Spintronics and quantum computing in nanostructures

S: Mesoscopic superconductors and hybrid structures	
Chair: Carlo Beenakker	
Olivier Buisson	Quantum dynamics of a current biased DC-SQUID
Paul Warburton	Nano-scale $1D$ arrays of intrinsic Josephson junctions
Bernard Pannetier	Cooper pair transport in an array of Josephson nano-junctions with dice lattice
Venkat Chandrasekhar	Thermopower in Andreev interferometers: Supercurrents and persistent currents
Fernando Sols	Entangled electron current through NS interfaces
Wednesday 8th	
F: Spin-dependent transport and control I	
Chair: Bryan Gallagher	
Laurens Molenkamp	Spin injection and detection in semiconductor spintronics
Bart van Wees	Spin injection, spin transport and spin manipulation in mesoscopic systems
Albert Fert	Spin injection and spin transfer experiments
Arne Brataas	Spin-battery operated by ferromagnetic resonance
F: Spin-dependent transport and control II	
Chair: Bart van Wees	
Xenophon Zotos	Ballistic transport in bulk 1D electronic/magnetic systems
Dietmar Weinmann	Spin dependent transport through magnetic domain walls in nanowires
Giancarlo Faini	Magnetization reversal in Co/Cu/Co pillars by spin injection
Andre Geim	Domain walls in the Peierls potential
S: Quantum manipulation and Qubits I	
Chair: Laurent Lévy	
Hans Mooij	Superconducting flux Qubits
Cristian Urbina	Operation of a solid state Qubit circuit
Lieven Vandersypen	Electron spin Qubits in quantum dots
S: Quantum manipulation and Qubits II	
Chair: Göran Wendin	
Per Delsing	Coherent oscillations in a single Cooper pair box
Yuriy Makhlin	Noise and dephasing in Josephson Qubits
Rosario Fazio	Decoherence in a Cooper pair shuttle

Thursday 9th	
S: Proximity, hybrid structures, mesoscopic superconductivity	
Chair: Hans Mooij	
Fabio Beltram	Quasi-particle ballistic transport in hybrid (and other) nanostructures
Frank Hekking	Measurement of coherent charge transfer in an adiabatic Cooper pair pump
Victor Petrashov	Electron transport in hybrid metallic nanostructures
T: Quantum of transport, statistics and noise	
Chair: Bernhard Kramer	
Boris Muzykantskii	Quantum statistics of non-equilibrium Fermi gas
Maura Sassetti	Spin and shot noise effects in 1D quantum dots
Klaus Richter	Spin control and spin relaxation in mesoscopic transport
Dominique Mailly	Quantum coherence in GaAlAs lattices: Evidence for Ahronov-Bohm cage effect
Closing of the meeting	

Section D: Physics of Quantum Dots

Coherent transport and electronic correlations in magnetic nanodevices

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Magnetic materials seem to be very promising for potential applications in future electronics. In such devices one can use both the charge and the spin degrees of freedom. We would like to present our recent studies [1,2] of the electronic transport in magnetic nanostructures, showing interplay of the both degree of freedom and a role of electronic correlations. The coherent transport will be considered, for which the typical quantum phenomena like interference (with the Fano resonance) or quantum many body effects like formation of Kondo resonance can be observed. The challenging problem is how these phenomena are influenced by finite magnetic polarisation of electrodes. The question of the stability of the singlet Kondo ground states appears and the possibility of additional control of magnetoresistance by polarisation of the leads arises.

In our theoretical studies we use the mean-field slave-boson and the equation of motion approach adapted for the non-equilibrium situation, within which electronic correlations and quantum interference processes are taken into account on the same level. Interference effects are pronouncedly seen in transport through the metallic ring with the quantum dot in the magnetic field, where the Aharonov-Bohm effect occurs together with the Kondo resonance. We predict that one should observe continuous evolution of the current characteristics with the magnetic

flux. For the system with the magnetic electrodes we show that the transport is uncorrelated in the empty state regime and the Julliere formula for the magnetoresistance is recover. In the Kondo regime the conductance tends to the unitary limit and the singlet state is formed, for which the spin accumulation reaches zero. The magnetoresistance is reduced due to electron correlations and it can even negative for strong asymmetry of couplings with the electrodes. For the mixed valence regime we predict a large magnetoresistance, which should exhibit a strongly temperature dependence.

[1] B.R. Bulka and P. Stefanski, Phys. Rev. Lett. **86**, 5128 (2001).
[2] B.R. Bulka and S. Lipinski, Phys. Rev. B, in press, January 2003.

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SU(4) Fermi liquid state in a Double Quantum Dot System

Jan von Delft

Universität München

We study a symmetrical double quantum dot (DD) system with strong capacitive inter-dot coupling using renormalization group methods. The dots are attached to separate leads, and there can be a weak tunneling between them. In the regime where there is a single electron on the DD the low-energy behavior is characterized by an SU(4)-symmetric Fermi liquid theory with entangled spin and charge Kondo correlations and a phase shift $\pi/4$. Application of an external magnetic field gives rise to a large serial negative magneto-resistance and a crossover to a purely charge Kondo state in the charge sector with SU(2) symmetry. In a four lead setup we find perfectly spin polarized transmission.

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Kondo physics on single and electrostatically coupled quantum dot systems

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Electrical transport through quantum dots is usually dominated by Coulomb blockade and single-electron tunneling. However, under certain circumstances a correlated state is formed between quantum dot and its leads, decribed in the framework of Kondo physics: The Coulomb blockade breaks down with lowering the temperature and the quantum dot becomes conductive like a one-dimensional channel. In the simplest case, the base for the description of this phenomenon is the so-called Anderson impurity model where usually a spin-degeneracy is assumed for the occupation of the quantum dot site by one electron and double-occupation is suppressed by Coulomb interaction. Two electrostatically coupled quantum dots – each with its own separate

leads – can be considered as a spin-less representation of the Anderson impurity model. Due to the electrostatic interaction such an arrangement demonstrate synergetic behaviour. In this talk experimental results on single and electrostatically coupled quantum dot systems will be presented.

References:

J. Schmid, J. Weis, K. Eberl, K. v. Klitzing, Phys. Rev. Lett. **84**, 5824 (2000).
M. Keller, U. Wilhelm, J. Schmid, J. Weis, K. v. Klitzing, K. Eberl Phys. Rev. **B 64**, 033302 (2001).
U. Wilhelm, J. Schmid, J. Weis, K. v. Klitzing, Physica **E 9**, 625 (2001).
U. Wilhelm, J. Schmid, J. Weis, K. v. Klitzing, Physica **E 14**, 385 (2002).

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Transport through Quantum Rings and Dots

Rolf J. Haug

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Small quantum rings and dots were produced in GaAs/AlGaAs heterstructures by direct writing with an atomic force microscope [1] and by electron-beam lithography. Aharonov-Bohm oscillations with up to 50 percent modulation are observed in the quantum ring in the case of one to two channel transport.
The quantum ring can be tuned from this open regime into the Coulomb-blockade regime in using in-plane gates. For small numbers of electrons in the ring a new periodicity appears as function of magnetic field [2].
The tunability allows for the observation of Fano and Kondo effects in transport through the quantum ring. These effects test the coherence of the system. In addition, the spin structure of the ring is tested via the Kondo effect. Kondo and Fano effects are also observed in a quantum dot with a large number of electrons [3]. Coupled-quantum dots are investigated in addition.

[1] J. Regul et al., Appl. Phys. Lett. **81**, 2023 (2002)
[2] U.F. Keyser et al. cond-mat/0206262
[3] C. Fühner et al., Phys. Rev. B **66**, 160305 (2002)

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Two-electron quantum dots as scalable qubits

J.H. Jefferson, M. Fearn, D.L.J. Tipton

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T.P. Spiller

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Two electrons confined in a square semiconductor quantum dot have two isolated low-lying energy eigenstates and hence the potential to realise scalable quantum computing elements (qubits). We show that this is indeed possible in principle by demonstrating that such elements can be initialised and made to perform the necessary single and two qubit transformations, using electrostatic gates and magnetic fields. Issues involving readout, decoherence, scalability and controlling entanglement via the Coulomb interaction will also be discussed.

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Coherent Transport and Electronic Interactions in Quantum Dots

Jörg P. Kotthaus

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Coherent transport of electrons is studied in quantum dot molecules defined electrostatically within GaAs heterostructures. In addition to single electron tunneling we observe correlated tunneling of two electrons in the regime where the exchange of electrons between the two quantum dots forming the molecule dominates the coupling of the quantum dots to the leads [1]. This cotunneling mechanism enables us to probe the spectrum of molecular states with little invasion as a function of the exchange coupling. In quantum dots defined by etched indentations in suspended GaAs heterostructure wires [2] we observe a suppression of conductance oscillation at low temperatures, low source-drain bias and low magnetic fields which we trace to the modified electron-phonon interaction in the suspended phonon cavity [3]. Here the recoil of the tunneling electrons can efficiently excite localized phonon modes and thus cause a phonon-mediated blockade of single electron transport.

[1] A. W. Holleitner, R. H. Blick, A. K. Hüttel, K.Eberl and J. P. Kotthaus, Science **297**, 70 (2002)

[2] E. M. Höhberger, R. H. Blick, F. Beil, W. Wegscheider, M. Bichler and J. P. Kotthaus, Physica E **12**, 487 (2002)

[3] E. M. Höhberger, J. Kirschbaum, R. H. Blick, T. Brandes, W. Wegscheider, M. Bichler, J. P. Kotthaus, to be published

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Angular Momentum and Spin Effects in Quantum Rings

Klaus Ensslin

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The experimentally detected energy spectrum of many-electron quantum rings can be understood on a quantitative basis. The circular symmetry in combination with only a few radially

occupied modes allows to identify levels which are basically governed by a single angular momentum quantum number. Here we set out to explore the spin degrees of freedom in quantum rings with the goal for an understanding and control of individual spin states.

The sample is fabricated by direct local oxidation of the surface of a GaAs heterostructure with a two-dimensional electron gas 35nm below the surface. In addition the homogenous top gate electrode greatly reduces interaction effects in the ring. This prerequisite allows the detailed analysis of spin pairs.

For magnetic field oriented in the plane of the sample the Zeeman splitting in the quantum ring is investigated. This allows us to characterize the spin sequence of electrons successively filling the orbital states of the ring.

By adjusting the gate voltage (and magnetic field) coupling strength, angular momentum and spin of the current carrying level can be selected. This tunability is unique to our system because of the excellent radial symmetry, which makes quantum rings excellent candidates for spintronics-based devices.

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Kondo effect in a quantum antidot in the quantum Hall regime

M. Kataoka, C.J.B. Ford, M.Y. Simmons, D.A. Ritchie

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We have observed Kondo behaviour between Aharonov-Bohm conductance resonances in individual quantum antidots at moderate perpendicular magnetic fields (B 1T). When edge states of the two spins of the lowest Landau level form bound states around the antidot, the resonances through these states show odd/even behaviour as B is varied. The odd/even effect vanishes when the temperature or the source-drain bias is increased. This behaviour is very similar to the Kondo effect in quantum dots, but it is not clear why it should occur in antidots. We have already shown that an antidot in the quantum Hall regime can be interpreted as a Coulomb-blockaded system - the charge in its vicinity can only relax in units of the electronic charge e, because the states are quantised and electrons can only be removed one by one. The coupling to the edge states in the leads can be tuned by gate voltage or field to change the strength of the effect, and hence the Kondo temperature.

The presence of the Kondo effect implies that in this regime two states with opposite spins are nearly degenerate even at non-zero B. In conjunction with a detailed analysis of the line-shapes, this may give information about the nature of the states around the antidot.

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Solid-state Structures for Quantum Information Processing

David A. Williams

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A number of new ways of manipulating information, generically known as quantum information processing, have been postulated in the last 15-20 years. Several have been demonstrated experimentally, but there remains a large gap between principle and practice, particularly in quantum computation. The success of solid-state electronics and optoelectronics in classical information processing leads many to the conclusion that condensed matter systems will provide the best way of bridging this gap. I will describe some of our approaches to making solid-state structures for quantum information processing, including nanoscale silicon and III-V semiconductor devices, carbon nanotubes and superconducting bridges. I will show recent experimental results, and discuss the various mechanisms which help and hinder the development of this field. There has been substantial progress in the last year, and I will give our view of the routes to making usable structures, particularly emphasising the many areas where an improved theoretical understanding would greatly assist progress.

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Section F: Ferromagnetic Junctions and Diluted Magnetic Semiconductors

Collective and Quasiparticle Properties of Semiconductor and Metallic Ferromagnets

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I will discuss the interplay between collective and quasiparticle properties of (III,Mn)V ferromagnetic semiconductors, arguing that in these systems spin-orbit interactions in the semiconductor valence band play an essential role in establishing the magnetic stiffness that permits itinerant electron ferromagnetism to occur at temperatures surprising close to the Fermi energy. I will also discuss phenomena like mangnetoresistance, in which quasiparticle properties are altered by adjusting the system's magnetic state, and inverse phenomena, like current-induced magnetization reversal in which the magnetic state is altered by adjusting the quasiparticle state, mentioning similarities and differences between metallic and semiconductor cases.

References: J. Konig, J. Schliemann, T. Jungwirth, and A.H. MacDonald, in *Electronic Structure and Magnetism of Complex Materials*, edited by D.J. Singh and D.A. Papaconstantopoulos (Springer Verlag 2002), [Also available at http://arXiv.org/abs/cond-mat/0111314]. See http://unix12.fzu.cz/ms/index.php for further references and a large database of theoretical predictions for magnetic, transport, and optical properties of ferromagnetic semiconductors.

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On the Electronic State of Mn Impurities in III-V Semiconductors

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Most phenomenological models of ferromagnetism in Mn doped GaAs assume that the Mn^{2+} impurity substitutes primarily the Ga^{3+} cation with five occupied majority d orbitals that have atomic character and a delocalized Hydrogen like acceptor state. While these assumptions are generally thought to be in agreement with experiment, they are presently not supported by ab initio electronic structure calculations. The latter, which are typically based on the Local Spin Density Approximation (LSDA) to Density Functional Theory, find the Mn d orbitals to be strongly hybridized with the As p states. In this picture the acceptor level is localized with substantial d-character. It is well known that due to spurious self-interactions LSDA calculations tend to overestimate the hybridization of such impurity states. In the present work we have performed first principles electronic structure calculations of Mn impurities in various III-V hosts using the Self Interaction Corrected Local Spin Density Method (SIC-LSD). The method is self interaction free by construction and reproduces the LSDA in the limit of delocalized states. Our calculations show that the electronic state of Mn is strongly affected by the SIC. In GaAs we find that all five Mn d-orbitals SIC correct leaving Mn in a d^5 state with a delocalized hole in the As p-band. When Mn substitutes Ga in GaN and GaP, the nature of the electronic state is quite different. Only four d-orbitals SIC correct leaving Mn in a d^4 state with a localized hole. These results seem to be in agreement with conclusions drawn from ESR experiments [1,2] and help settle the discussion over the electronic state of Mn in GaP [3]. Moreover the present results imply that the exchange mechanism between Mn moments and must be different for different III-V host systems.

[1] Schneider et. al. Phys. Rev. Lett. **59**, 240 (1987);
[2] Kreissl et al. Phys. Rev. B **54**, 10508 (1996);
[3] Dietl et al. cond-mat/0109245.

Work supported by the Defense Advanced Research Project Agency and by DOE Office of Science through ASCR/MICS and BES/DMSE under Contract No. DE-AC05-00OR22725 with UT-Battelle LLC.

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Excitons in self-assembled type II quantum dots and coupled dots

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Excitons in a type II quantum dot are studied in the presence of a perpendicular applied magnetic field. The dot is modelled by a quantum disk with radius R, thickness d and the electron (hole)

is confined in the disk, whereas in the unstrained case the hole (electron) is located in the barrier. The exciton energy and wavefunctions are calculated using a Hartree-Fock mesh method. The results are applied to the InP/GaInP self-assembled quantum dot system.

For sufficient wide and thin dots, the strain field leads to a confinement of the heavy hole within the dot and the system is type I, while the light hole is confined outside the dot leading to a type II light exciton. With increasing disk thickness, the strain induces a transition of the heavy hole from inside the disk towards the radial boundary outside the disk. We predict a heavy-hole to light-hole exciton transition as a function of the disk thickness. There is a range of parameters (disk thickness and radius) for which a magnetic field is able to induce such a transition.

The present system exhicits a rich physics with: i) angular momentum transitions as function of the magnetic field, ii) a large linear Stark effect in contrast to the well-known parabolic Stark effect in type I dots, iii) spontaneous symmetry breaking of the exciton state in coupled dots, and v) magnetic field induced dipole moment of the exciton.

Work done in collaboration with: K. Janssens, B. Partoens and M. Tadic.
This work was published as: Phys. Rev. B **64**, 155324 (2001); **65**, 165333 (2002); **65**, 233301 (2002); **66**, 075314 (2002); Physica E **12**, 880 (2002); **13**, 237 (2002); J. Appl. Phys. **92**, 5819 (2002).

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Transport properties of diluted magnetic semiconductor ferromagnets

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In some metallic (III,Mn)V compounds the microscopic origins of ferromagnetism are already well understood and efficient computation methods have been developed to model their magnetic, transport, and optical properties. In this contribution we discuss theoretical results for the anomalous Hall effect, anisotropic magneto-resistance, and the infrared ac-transport coefficients that describe quantitatively many of the experimental properties of (Ga,Mn)As ferromagnetic semiconductors.

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Magnetotransport in high quality Ferromagnetic Ga1-xMnxAs

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We present results for high quality ferromagnetic $Ga_{1-x}Mn_xAs$ grown by MBE using As_2 and procedures to minimise defect densities. We find that post growth annealing of thin epi-layer

leads to Curies temperatures of up to $151K$. this is considerably higher than the long standing record value of $110K$. Excellent structural quality is demonstrated by high resolution X-Ray diffaction studies in which the reduction of defect density resulting from the use of As_2 is demonstrated. We obtain metallic conductivity over a wider range of Mn compositions than has previously been achieved (1.5% to 8%) and conductivities which are considerably lower than previously published result.

The low resistivities of our samples is accompanied by very low magnetoresistances. This enables us to separate the normal and anomalous contributions to the Hall effect.

We also demonstrate that it is possible to extract hole densities to a high degree of accuracy for these samples. We find that for the annealed samples, which have the highest Curie temperatures, that hole density is approximately equal to the Mn concentration. We find that the Curie temperature are reasonably well accounted for by the predictions of the mean field theory.

We present a detailed study of the resistivity-dependence of the anomalous Hall effect at high magnetic fields and low temperatures. The anomalous Hall coefficient is shown to have a predominantly quadratic dependence on the resistivity and a magnitude which is a good agreement with the Berry phase theory of the anomalous Hall effect [3].

We also report the observation of a large aniosotropic magnetoresitance in our samples which are consistent with recent calculations, and demonstrate the existence of uniaxial anisotropy in our samples.

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Magnon-assisted transport in ferromagnetic junctions

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We present a theoretical description of the thermopower due to magnon-assisted tunnelling in a mesoscopic tunnel junction between two ferromagnetic metals [1,2]. The thermopower is generated in the course of thermal equilibration between two baths of magnons, mediated by electrons. For a junction between two ferromagnets with antiparallel polarizations, the ability of magnon-assisted tunneling to create thermopower S_{AP} depends on the difference between the size $\Pi_{\uparrow,\downarrow}$ of the majority and minority band Fermi surfaces and it is proportional to a temperature dependent factor $(k_BT/\omega_D)^{3/2}$ where ω_D is the magnon Debye energy. The latter factor reflects the fractional change in the net magnetization of the reservoirs due to thermal magnons at temperature T (Bloch's $T^{3/2}$ law). In contrast, the contribution of magnon-assisted tunnelling to the thermopower S_P of a junction with parallel polarizations is negligible. As the relative polarizations of ferromagnetic layers can be manipulated by an external magnetic field, a large difference $\Delta S = S_{AP} - S_P \approx S_{AP} \sim -(k_B/e) f(\Pi_\uparrow, \Pi_\downarrow)(k_BT/\omega_D)^{3/2}$ results in

a magnetothermopower effect. This magnetothermopower effect becomes giant in the extreme case of a junction between two half-metallic ferromagnets, $\Delta S \sim -k_B/e$.

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Spin injection and spin accumulation in a mesoscopic metal island

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In a spin valve experiment, the basic idea is to create a spin imbalance into a non magnetic metal or semiconductor. Spin injection from FM electrodes into a diffusive paramagnetic metal has been shown both for clean contacts (FM/N) and with tunnel barriers (FM/I/N) [F.J. Jedema *et al.*, Nature **410**, 345 (2001), F.J. Jedema *et al.*, Nature **416**, 713 (2002)]. As the Al strip is much longer than the spin flip length, the spins diffuse in the metal and can "leak out", and eventually relax, undetected.

Following this work, we study spin injection into an island whose size ($500\times500\ nm^2$) is smaller than the spin relaxation length $\lambda_{sf} \approx 1\mu m$. This results in the spin imbalance being uniform in the island. Moreover, as the spin accumulation scales with the volume of the metal, one expects the spin signal to increase compared to the previous experiments.

Figure 1 shows a SEM picture of the sample. Four FM electrodes are connected to the island in order to perform a 4-terminal measurement: this allow us to separate the voltage probes from the current path. By sweeping an externally applied magnetic field, we are able to change the magnetisation direction of the current electrodes from parallel to antiparallel. Only in the antiparallel case one observes spin accumulation. As the FM voltage probes are more sensitives to one of the two spin populations, we can electrically detect the spin imbalance. In the samples with tunnel barriers between FM electrodes and Al island, we achieve a spin dependent resistance of 0.3 Ω, which is about 25 times larger than previously observed.

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Spin injection and spin transfer experiments

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Injecting spins and exploiting the resulting spin accumulation is the basis of several spintronic devices. For example, spin accumulation can be used to transform a magnetic information into an electrical signal or to switch a magnetic configuration by spin transfer. After an introduction on

the physics of spin-injection and spin accumulation, I will focus on two types of experiment : 1) Spin injection into a GaAs quantum well (QW) with electrical detection of the spin polarization in the QW [1]. 2) Magnetization reversal of a ferromagnetic layer by injection of an obliquely spin polarized current and spin transfer from the current to the layer (experiments on Co/Cu/Co multilayered pillars) [2].

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Spin-battery operated by ferromagnetic resonance

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Precessing ferromagnets are predicted to inject a spin current into adjacent conductors via Ohmic contacts, irrespective of a conductance mismatch with, for example, doped semiconductors. This opens the way to create a pure spin source "spin battery" by the ferromagnetic resonance. We estimate the spin current and spin bias for different material combinations.

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Field dependence of the magnetic switching induced by a spin polarized current in Co/Cu/Co pillars: a probe for theoretical models.

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We present experimental results on the magnetization reversal driven by a spin polarized current in pillar-shaped Co 150 / Cu 100 / Co 25 trilayers. Besides experiments performed at zero field in agreement with previous results on similar pillars [1], we also study the field dependence of the critical currents and clearly evidence the existence of two regimes according to the amplitude of the applied field H_{app} compared to an anisotropy field H_{an}. For $H_{app} < H_{an}$, the reversals from parallel to antiparallel and vice versa, are sharp as the respective critical currents are

reached and the resulting $R(I)$ curve is hysteretic. For $H_{app} > H_{an}$, the reversals are much smoother and fully reversible. Up to now, two theoretical approaches have been proposed in order to calculate the current induced torque. The model based on a direct interaction between the magnetic moment carried by the conduction electrons and the local magnetization is unable to explain even qualitatively these later results [2]. On the contrary, we are able to interpret them correctly in the frame of the spin transfer model [3] using a diffusive approach. We present a detailed calculation of the spin polarization of the conduction electron using the Valet-Fert model developed for the CPP-GMR and the critical currents extracted from the Landau-Lifschitz-Gilbert equation in presence of an external applied field. The comparison with our experimental results leads us to the conclusion that only the spin transfer approach is able to describe properly the properties of the spin current induced magnetization reversal.

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a) On leave from the Department of Physics, Faculty of Science, HR-10000 Zagreb, Croatia.

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Domain walls in the Peierls potential

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We report on how individual domain walls in a ferromagnet move on a scale less than its interatomic spacing and interact with the underlying crystal structure, which is usually referred to as the Peierls potential. In our experiments, ballistic Hall micromagnetometry was employed to resolve small changes in a local magnetic field, which are induced by changes in the average position of micron-sized segments of domain walls in samarium-yttrium-iron garnet. The ferromagnetic garnet has strong magnetic anisotropy at low temperatures, which results in its domain walls being extremely narrow ($\approx 10nm$) covering only several periods of the crystal lattice ($1.2nm$). We have found that such domain walls propagate through the garnet crystal in discrete jumps of the same length matching the lattice periodicity. We believe that it is the first direct observation of an object moving in the Peierls potential.

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Section M: Nanoelectronic Materials and Interfaces

Magnetism under the Microscope

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In the field of magnetoelectronics and spintronics one deals with a large variety of thin ferromagnetic films consisting of transition-metals, half-ferromagnets, or magnetic semiconductors whose properties may change substantially when restricted to low dimensions or in contact with non-magnetic spacer layers, antiferromagnetic bias layers, oxide barrier films or semiconductor films. Depending on the growth condition these multicomponent junctions may exhibit complex magnetic spinstructures on different length scale. An overview is presented on the recent progress of ab-initio theory in combination with model theory in determining (i) new magnetic materials (ii) complex magnetic structures on the atomic scale [1], (iii) how these magnetic structures may be revealed using a spin-polarized scanning tunneling microscope [2,3], (iv) how the spin-orbit dependent tunneling cross section can be used to detect magnetism with a conventional STM [4], and the tunneling through semiconductor and oxide barriers. The ab-initio calculations are based on the density-functional theory and are carried out with the full-potential linearized augmented plane wave method (FLAPW) or the Green-function Korringa-Kohn-Rostocker (GF-KKR) method.

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Half-metallic transition metal oxides

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In this talk we briefly overview the characteristics and applications of half-metallic ferromagnets. We discuss an application of the self-interaction corrected local spin density approximation (SIC-LSD) to some half-metallic compounds, and among them the double perovskites Ba_2FeMoO_6, Ca_2FeMoO_6, Sr_2FeMoO_6, Ca_2FeReO_6, and magnetite (Fe_3O_4). We also mention briefly mixed valence manganite compounds, and show that also such simple transition metal monoxides as NiO and MnO can show half-metallic characteristics when doped with vacancies. In the double perovskites we concentrate on the electronic and magnetic properties of these compounds and in particular the size and relative orientation of the spin moments of Fe and Mo or Re. In all the compounds the calculations find a spin moment of about 0.4 μ_B on the Mo sites and $\sim$1.0 μ_B on Re, with an opposite orientation to the respective spin moments on Fe sites. We find these double perovskites to be half-metallic, with a well defined gap in the spin-up density of states, and strong hybridization at the Fermi energy between the spin-down Fe $3d$, Mo $4d$ (or Re $5d$), and O $2p$ states. Issues of charge ordering in magnetite are also discussed. We find that the charge ordered phase is not the groundstate solution for this compound.

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Conductance of gated metal-molecule-metal nano-junctions

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One of the major challenges on the road to molecular electronics is to organize the molecular building blocks into micro- and eventually macroscopic circuits. Many different approaches to contact a small number of molecules have been developed the recent years. Some of the methods exploit the flexibility of tunable contacts to molecules afforded by scanning probes or break junctions. Other methods use a fixed contact arrangement. We employ new techniques that combine some advantages of both tunable and fixed contacts. The methods are similar to the fabrication of single-electron transistors using the shadow angle evaporation. The device performance can be monitored during fabrication as with tunable contacts, but the contact geometry is fixed, providing good mechanical and thermal stability. Based on our ability to measure the conductance from the earlier stages of molecular junction formation and the scanning probes studies of monolayers of conjugated molecules I discuss the importance of the microscopic control of the molecule-metal interfaces, including the surface topography of the metal, formation of chemical bonds at the interfaces, surface diffusion, granularity, contamination and/or oxidation.

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TranSIESTA: A SPICE for Molecular Electronics

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With our newly developed method, TranSIESTA[1], it has become possible to model complex molecular electronics devices under operation conditions. In this presentation I will describe the basic principles behind the method and applications of the method to model recent experimental data for molecular rectifiers and molecular devices displaying negative differential resistance.

The TranSIESTA method is based on density functional theory, and calculates the selfconsistent electronic structure of a molecule coupled to 3-dimensional electrodes with different electrochemical potentials, using a full atomistic ab initio description of both the electrodes and the molecular structure. The calculations reveal information about the scattering states, transmission coefficients, electron current and nonequilibrium forces in the system.

We have used the method to investigate the IV characteristics of an Aviram-Ratner type molecular diode and compared the theoretical results with experimental data. The calculations reveal that the electrode coupling plays an important role, and that an asymmetric coupling to the external electrodes is the origin of the rectification observed experimentally. To investigate the effect of electrode coupling we have calculated the IV characteristics of a symmetric molecule,

a phenylene-ethynylene oligomer, for different electrode couplings. From these calculations we extract a simple model for the diode characteristics as function of the molecular coupling to the external electrodes.[3] These relations can rationalize several experimental results, and may be used to design molecular diodes with improved properties.

Other experiments of Phenylene-ethynylene with nitro side groups[4] have shown Negative Differential Resistance. We have calculated the IV characteristics of Phenylene-ethynylene oligomers with a varity of sidegroups, and based on these calculations we discuss the origin of the complex electrical behaviour of these systems.

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Assembly and Processing of Molecular Nanostructures

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Recent experiments on the organisation of molecules both by direct manipulation using the tip of a scanning tunnelling microscope and also through spontaneous assembly mediated by hydrogen bonding centres are discussed. Manipulation of large molecules, such as C60, on semiconductor surfaces has been found to be possible at room temperature in both attractive and repulsive mode. Manipulation is also possible if the fullerene cage is modified through the incorporation of N atom and also for endohedral fullerenes. However attachment of sidegroups inhibits manipulation suggesting a rolling mechanism in which translation and rotation are coupled. Alternative methods for assembling molecular structures based on directional intermolecular interactions such as hydrogen bonding have also been investigated. Imide derivatives of NTCDA and PTCDA, materials investigated in relation to molecular electronics, interact to form chains, islands and complex networks. These structures are sufficiently cohesive to be displaced using a scanning tunnelling microscope and have a stability which depends on commensurability with an underlying lattice. The exploitation of hydrogen bonding to form more complex networks is also discussed.

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Theoretical modeling of DNA-based biomolecular nanowires

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The search for novel efficient molecular nanowires based on DNA derivatives, and their experimental and theoretical characterization, lies at the core of Molecular Electronics. By virtue of their recognition and self-assembling properties, as well as of their mechanical stability, DNA molecules seem particularly suitable as the active components for nanoscale electronic devices. However, whereas it was demonstrated that the self-assembling capabilities of DNA might be used to wire metallic materials in a programmable way [1], its ability as an intrinsic conductor is questioned by various experimental results [1,2]. Depending on base sequence, molecule length, ambient conditions, substrates, electrode materials, experiments for the direct measurement of the dc conductivity in DNA-based structures report insulating character [1,2], semiconductor-like transport characteristics [3], ohmic behavior [4], and even proximity induced superconductivity [5]. Such a huge discrepancy might eventually be solved by choosing to investigate well-defined molecular structures, for instance by restricting the base sequence. Among the bases of DNA, guanine (G) is particularly interesting for the possibility to synthesize conductive molecular aggregates, because of its low ionization potential, which suggests its viability to mediate charge motion along a strand. In this presentation, we first discuss band structure features of model single-stranded guanine stacks and their dependence on the rotation angle between consecutive bases [6], and then focus on tubular sequences of G-quartets (G4), whose formation is known to be driven by alkali cations. G4 quadruple helix nanowires consist of stacked planar hydrogen-bonded guanine tetramers. Our investigations are based on plane-wave pseudopotential DFT calculations of periodic structures. Concerning G4, our results [7] show that long wires form and are stable with incorporation of metal ions. We present their electronic band structure and discuss the interpretation in terms of effective wide-bandgap semiconductors. In spite of the localized character of the electron wave functions (due to the poor π-π superposition [6]), the calculated density of states is consistent with a model of a semiconducting nanowire, which hosts effective channels for electron/hole mobility.

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Nanoelectronics with Carbon

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The electronic structure of carbon-based nanotubes is now well established. Ballistic conductance behavior observed in carbon nanotubes derives from the crossing of two conduction bands at the Fermi point. Unexpected transport behavior can arise from the changes in the electronic structure at the Fermi level when such nanotubes are deformed, or when their chemical composition is changed. The competition between the Fermi surface deformation due to an applied magnetic field and a structural twist may lead to an unexpected giant magnetoconductance in carbon nanotubes [1]. In heterostructured nanotubes, partly filled states at the interface of carbon and boron nitride segments may acquire a permanent magnetic moment. Depending on the atomic arrangement, artificially formed C/BN superlattices may exhibit an itinerant ferromagnetic behavior [2]. In other all-carbon nanostructures, presence of carbon radicals may lead to ferromagnetic behavior with a high Curie temperature [3], an important step in the direction of spintronics.

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Electrical measurements on phenylene-based conjugated molecules

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For both fundamental reasons and possible electronic applications, there is a big interest in measuring and understanding electron transport across organic molecules. However, due to the immense challenges in contacting nanometer-sized objects, a coherent picture has not yet emerged. Here we add to the experimental data and present results on measurements of phenylene-based organic molecules with sizes between 1 and $10nm$. A three-terminal device geometry was employed with a thin native aluminium gate oxide to achieve as high gate effects as possible. The long molecules were connected to prefabricated gold electrodes with gaps between 5 and $10nm$, while the short molecules were first made to form self-assembled monolayers on one electrode before evaporating the second electrode on top. None of the molecules investigated showed a strong gate effect. However, a weak gate effect could be observed for a $10nm$ long molecule.

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Ab-intio study of the magnetoresistance effects in magnetic nanocontacts

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Using the first-principle screened Korringa-Kohn-Rostoker (SKKR) method for the electronic structure calculations we have investigated transport properties of atomic sized nanocontacts. We have modeled the nanocontacts by short atomic chains of Co, Cu, Al and Si atoms embedded between magnetic semi-infinite Co(100) leads. The Landauer formalism adapted for the SKKR method was used to calculate conductance and magnetoresistance (MR) as a function of the electron energy in the region $-1.5eV \ldots +1.5eV$ nearby the Fermi level. We found that magnetic leads result in a complicated energy dependence of the minority conductance both for magnetic Co chains and chains formed from nonmagnetic (Cu, Al, Si) atoms. It will be shown that MR is sensitive to geometry and chemistry of the constriction. MR ratios of $20 - 50\%$ are obtained for Co, Cu, Al and Si chains between Co leads at the Fermi energy. MR ratios even higher than 50% are obtained for energies about $-0.3eV$ below the Fermi level.

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FFLO State in Ferromagnet - Superconductor Heterostructures

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I shall discuss the ground state properties of a 'ferromagnet - superconductor' heterostructure on the basis of a semiclassical theory featuring exchange splitting in the ferromagnet and electron - electron attraction in superconductor. We have solved the spin - polarized Eilenberger equations together with the Maxwell's equation (Ampere's law) fully self-consistently. We have found that due to proximity effect the Fulde - Ferrel - Larkin - Ovchinnikov ($FFLO$) - like state [1,2] is realized in such a heterostructure. It manifests itself in oscillatory behavior of the pairing amplitude in FM and spontaneously generated current (and magnetic field) in the ground state of the system [3,4]. I shall discuss the presence of the Andreev bound states, the position of which can be tunned either by exchange splitting or by thickness of the ferromagnet, and its relation to the current and the pairing amplitude. I shall also show how the elastic disorder and finite transparency of the interface influence the $FFLO$ phase in the system.

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Spin transport from first principles

Paul J. Kelly

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Interfaces play a crucial role in nanoscale electronic devices. The spin-dependence of electronic transport across an interface is an essential element in understanding giant magnetoresistance in layered metallic structures and related effects such as point contact Andreev reflection at Ferromagnet/Superconductor contacts. We have developed a method based on first-principles density functional theory and the tight-binding linear-muffin-tin orbital surface Green's function method to calculate the spin-dependent interface resistances for interfaces such as Co/Cu, Fe/Cr, Cu/Ag and Cu/Nb. Disorder is treated by means of large lateral supercells. Without introducing any free parameters, quantitative agreement with experiment is obtained. Even ideal interfaces can have very low transmission which may be increased by disorder.

Work carried out in collaboration with G.E.W. Bauer, S. Gerritsen, M. Talanana, I. Turek, K. Xia, and M. Zwierzycki

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Transport, forces and vibration modes in a chain of single gold atoms

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Using STM techniques we fabricate freely suspended atomic chains of single gold atoms at liquid helium temperatures. These chains, which form spontaneously during the fracture of gold nanocontacts [1], form very stable metallic wires. Using a very senstitive force sensor we can resolve the force evolution during the formation of the chain, where the individual atomic-rearrangement events for addition of atoms to the chain can be clearly identified [2]. We find that the bond strength of the chain is about twice that of a bulk metallic bond. Electronic transport in these chains is ballistic and takes place through an almost completely open conductance channel giving a conductance very close to $2e^2/h$. Using point-contact spectroscopy, we study the vibration modes of these chains [3,4]. Compared to the bulk vibration spectrum of gold the transverse accoustic phonons are absent, and the frequency of the longitudinal accoustic phonons can be tuned by varying the tensile force on the chain.

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The electron spin in carbon nanotubes

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Metallic single wall carbon nanotubes are typically $1nm$ diameter and $1\mu m$ long ballistic wires. Orbital energies for the electrons have therefore almost atomic (eV) values and the spin of the electrons therefore represents the only relevant angular momentum. For this reason and because of the simple one-dimensional energy spectrum, the effect of spin is readily observable in a number of experiments. The spin most immediately enter into the single electron transistor experiments as an even-odd phenomenon and in the Zeeman splitting in a magnetic field. In a more subtle way a spin $\frac{1}{2}$ state may lead to a co-tunneling, which takes advantage of the spin-degeneracy (Kondo-resonance) and possibly in the creation of a new Luttinger state of the one-dimensional electron gas. The spin state of the single wall carbon nanotube also has a bearing on the superconducting and magnetic proximity affect into the tube. Neutral impurity with non-zero spin placed inside or outside the nanotube may also be recognizable by its spin $\frac{1}{2}$ state.

Carbon Nanotube Quantum Dot with Superconducting Leads

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Carbon nanotubes (CNTs) can serve as model systems for the exploration of transport phenomena in low-dimensions. Here, we report on electric transport through CNTs quantum dots (zero-dimensional regime) using multi-wall CNTs (MWNTs). While transport through a quantum dot is governed by the phenomenon of single-electron charging if the dot is weakly coupled to the leads, higher-order tunneling processes (so-called co-tunneling) significantly add to the electrical current at moderate to high lead couplings. This latter regime will be the focus of the presentation. It is characterized by many-electron processes, the most prominent of which is the Kondo effect. We have observed the Kondo effect in transport through MWNTs [1] and moved on to explore the interplay between superonducting proximity effect and Kondo physics.[2] This is realized by using superconducting leads (Al). Non-linear transport reveals sub-gap peaks, characteristic for multiple Andreev processes. In (or near equilibrium) the Kondo effect (the Kondo resonance) can coexist with superconductivity in the leads, provided the Kondo temperature is larger or of similar magnitude than the superconducting order parameter. In the opposite limit, the onset of superconductivity suppresses the conductivity.

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Section S: Mesoscopic Superconductors and Hybrid Structures

Current Amplifier based on a Mesoscopic Josephson Junction

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Quantum dynamics of a Josephson junction can be utilized to construct low-noise transistor-like amplifiers, Bloch Oscillating Transistors (BOT), that have high input impedance $Z_{in} \cong 500$ kΩ, current gain $\beta \cong 30$, power gain $\eta \cong 5$, and noise temperature $T_N \cong 0.5$ K. The operating principle of a BOT is based on the fact that Zener tunneling up to a higher band will lead to blockade of Cooper-pair tunneling (Bloch oscillation) in a suitably biased Josephson junction. Bloch oscillation is resumed only after the junction has relaxed to the lowest band by quasiparticle tunneling. Thus, a small quasiparticle control current is able to control a much larger supercurrent component. These devices provide novel quantum-electronic building blocks that will be useful in low-noise, intermediate-impedance-level circuit applications at low temperatures. The experimental realization of BOTs and the first experimental results obtained on them will be discussed [1].

[1] Work done in collaboration with J. Delahaye, J. Hassel, R. Lindell, M. Sillanpää, M. Paalanen, and H. Seppä

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Theory of half-integer flux quantization in d-wave superconducting rings

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A.M. Martin

Nottingham University

Flux quantization with units of $\Phi_0 = h/2e$ in conventional mesoscopic superconducting rings is a consequence of the single-valuedness of the order parameter. However in unconventional superconductors it is possible to develop non-trivial textures in the superconducting order parameter, and hence various exotic topological defects. In the case of d-wave high Tc superconductors

half-integer flux quanta can occur in small rings containing one or more grain boundary Josephson junctions. We show that this effect is an intrinsic topological property of the ring geometry. By explicit self-consistent calculations of the spontaneous ground state current in small d-wave rings, we show that the current flow derives from splitting of a zero energy Andreev bound state. This topological and microscopic explanation for half-integer flux quantization can be contrasted with the usual interpretation in terms of grain boundaries which are either normal or 'pi' Josephson junctions.

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Shuttling of Single Electrons and Cooper Pairs

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The aim of the presentation is to emphasize the role of coupling between electronical , mechanical and possibly magnetic degrees of freedom, taking place on a nanometer length scale. Such coupling affects significantly electrical properties of nanocomposite materials which are usually heteroconducting and geteroelastic by their nature. An instability in selfassembled single electronic device and shuttling of electrical charge [1] by movable Coulomb dot, transferring of magnetization by movable nanomagnetic particle as well as shuttling of Cooper pairs [2,3] by movable Single Cooper Pair Box are discussed as examples of nanoelectromechanics in normal, superconducting and magnetic composites.

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Cooper Pair Tunneling and Coulomb Blockade

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One dimensional arrays of small capacitance Josephson junctions form an interesting system for the study of single Cooper pair transport in a high impedance environment. The arrays can be modeled as a transmission line with an impedance that can exceed the quantum resistance. In this case, a Coulomb blockade results, in spite of the very large Josephson coupling energy and

the low impedance of the environment (voltage bias of the array). The arrays can be fabricated in a SQUID geometry to allow for tuning of the Josephson coupling energy. Experiments will be described which investigate the Coulomb blockade regime in these arrays, and the use these arrays as a tunable electrodynamic environment for the study of tunneling in a single, small capacitance Josephson junction.

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Ferromagnetism and superconductivity in quantum dot arrays

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The flat-band ferromagnetism in quantum dot arrays is theoretically proposed [1]. By using a quantum dot as a building block, quantum dot superlattices are possible. By performing an exact diagonalization of the Hubbard Hamiltonian for the dot arrays on Lieb and Kagome lattices, we calculate the dot-size dependence of the energy difference in a dot model and estimate the transition temperature of the ferromagnetic paramagnetic transition, which is found to be accessible within the present fabrication technology.

We also study magnetic-field effects on the flat-band ferromagnetism on a Kagome lattice [2]. Application of a perpendicular magnetic field destroys the flat-band ferromagnetism and induces a metal-insulator transition because the flat band has a finite dispersion.

Based on calculations using the local density approximation, we propose quantum wire networks with square and plaquette-type lattice structures that form quantum dot superlattices [3]. Numerical analysis reveals a superconducting ground state with transition temperatures of up to 90 mK for the plaquette [4].

These phenomena, the flat-band ferromagnetism, the metal-insulator transition and superconductivity are found to be accessible within the present fabrication technology. In order to observe these phenomena we developed a new GaAs/AlGaAs heterostructure. Here we present preliminary studies on the electronic transport in a quantum dot based on a back-gated undoped GaAs/AlGaAs heterostructure. The quantum dot is well defined by means of a single metallic front-gate. We observe clear regions of Coulomb blockade and pronounced tunneling peaks in a broad range of source-drain and front-gate voltages. Excellent agreement to the calculated Coulomb diamond pattern using the constant interaction model is achieved if a front-gate voltage dependent change of the dot capacitance is taken into account.

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Hanbury Brown Twiss Effects in Channel Mixing Normal-Superconducting Systems

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Correlations of currents at different leads of normal conductors have recently been measured. These correlations can be viewed as an analog of the optical Hanbury Brown Twiss effect in optics. In hybrid normal-superconductors Andreev reflection leads to a rich behavior of these correlations. Initial work considered only single channel normal conductors connected to a superconductor. We are interested in structures with channel mixing [1,2] and discuss correlations for an ensemble of mesoscopic conductors. A wide range of geometries has been investigated for chaotic cavities: for good coupling to the superconductor and open normal contacts the proximity effect generates positive correlations [3]. These are suppressed and turn negative by application of a magnetic field equal to a single flux quantum through the cavity [3]. In the absence of the proximity effect, positive correlations result if Andreev scattering is suppressed with the help of a barrier between the cavity and the superconductor [3]. We explain this in terms of a pair partition noise and a pair breaking noise. In the absence of the proximity effect, for multichannel systems, we discuss a quasi-classical theory, both for second-order and higher order current correlations [4].

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Spectroscopy and decoherence in a double-island qubit

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We have probed by tunnel spectroscopy a quantum system consisting of two superconducting islands strongly coupled by an ultrasmall Josephson junction. The Josephson junction allows Cooper pair delocalization between the two islands and gate voltages control the state of the system. Tunnel spectroscopy is made possible by means of two other junctions weakly coupling

the islands to the tunneling electrodes. We have observed three distinct regime depending on the applied bias voltage:

1. When the electrostatic energies of both islands are close, the transport occurs by tunneling into the upper state of the qubit and out of the lower state.

2. Further away from degeneracy, transport occurs by cotunnelling across two junctions. An abrupt transition with the above process takes place.

3. At larger bias voltages, in spite of the presence of quasiparticles, transport still involves Cooper pairs and one family of energy levels of the double island can still be mapped.

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Pascal distribution of voltage fluctuations out of equilibrium

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The current–voltage or charge–phase duality plays a central role in quantum transport. It was studied originally in connection with superconducting Josephson junctions and more recently in the context of single-electron tunneling. Quantum mechanically, the duality appears because current I and voltage V are noncommuting operators. This is conveniently expressed by the canonical commutator $[\Phi, Q] = ie$ of the transferred charge $Q = \int_0^\tau I(t)dt$ and accumulated phase $\Phi = (e/\hbar)\int_0^\tau V(t)dt$ (in a given detection time τ). Moments of charge and phase determine the measured correlators of current and voltage, respectively.

While all moments of Q in a voltage-biased conductor are known (derived by Levitov and Lesovik in 1993), the dual problem (moments of Φ under current bias) has only been studied for the first two moments. The first two moments in the dual problems are simply related by rescaling $I(t) \to V(t) \times G$ (with G the conductance). One might surmise that this linear rescaling carries over to higher moments, so that the dual problems are trivially related. But is it true?

We have found that electrical noise becomes intrinsically different when the conductor is current biased rather than voltage biased. While the second cumulants can be related by a rescaling with the conductance, the third and higher cumulants can not. The non-linear term that breaks the rescaling is of the same order of magnitude as the linear term, so it can not be neglected. From a fundamental point of view, the limit of full current bias is of particular interest. The counterpart of the celebrated binomial distribution of transferred charge turns out to be the *Pascal distribution* (or "binomial waiting-time distribution") of phase increments.

Work done in collaboration with M. Kindermann (Leiden) and Yu.V. Nazarov (Delft).

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Cooper pair transport in an array of Josephson nanojunctions with dice lattice

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Charged particles on a dice lattice have been shown to exhibit an interesting localization (cage) effect [1] due to Aharonov-Bohm destructive interferences. This confinement effect takes place when the external magnetic field corresponds precisely to half a flux quantum per plaquette (frustration f=1/2). Recently some signatures of this effect were observed experimentally on mesoscopic systems consisting of artificial arrays made of either superconducting (Al, Nb) [2] or quantum (GaAs) wires [3]. He we present results on arrays of Josephson nanojunctions having the same dice lattice. The issue is to understand how Cooper pair transport is affected by the cage effect. We have fabricated a series of arrays in both the phase ($E_c < E_J$) and the charge regime ($E_c > E_J$). E_c is the charging energy and E_J the Josephson coupling energy for one junction. We find that Cooper pair transport is strongly modified in this lattice as compared to the square lattice. In the classical regime, we see evidence for a very weak commensurate state at f=1/2. We discuss the vortex correlations [4] and the possible occurence of the glassy state suggested in [5]. In the charge regime we observe the Coulomb blockade of Cooper pairs leading to a fully insulating state at f=1/2. In the intermediate regime a metallic state is observed down to the lowest temperature (less than 50 mK) and over a significant magnetic flux range. Also we find the Josephson coupling in this lattice surprisely robust against quantum fluctuations at zero magnetic field.

The e-beam lithography was carried out with CEA-LETI-PLATO organization teams and tools.

Work done in collaboration with E. Serret, F. Balestro, O. Buisson, K. Hasselbach and Th. Fournier

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Thermopower in Andreev Interferometers: Supercurrents and Persistent Currents

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The thermopower of Andreev interferometers shows oscillations as a function of the magnetic flux ϕ coupling to the loop, with a fundamental period of $\phi_0 = h/2e$, evidence of the quantum coherent nature of thermal transport in this mesoscopic size regime. The oscillations can be either symmetric or antisymmetric in ϕ, depending on the topology of the Andreev interferometer. I will describe our experiments on quantitatively measuring the thermopower of Andreev interferometers, and explain the unique interplay of electrical, thermal and the analog of normal-metal persistent currents that gives rise to these unusual symmetry properties.

This work was done in collaboration with Zhigang Jiang, Dima Dikin, and Jonghwa Eom, and was supported by the US National Science Foundation.

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Entangled electron current through normal-superconductor interfaces

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We study the tunneling current emitted from a BCS bulk superconductor into a bulk normal metal through an interface with a finite area. We restrict ourselves to the limit of vanishing temperature and voltage bias. We derive a local 3D tunneling Hamiltonian which accounts for the different hopping behavior at various electron energies. Based on the picture of two-electron emission, our predictions for the angular distribution of the current through an infinite interface are identical to those obtained by invoking the Andreev reflection mechanism. We provide a physical explanation for this equivalence. Our method can be used to address real space problems and realistic barrier shapes. We analyze the radial dependence of the density current for different contact radii and barrier heights, and identify several transport regimes. We also calculate the current through two small orifices at a certain distance. Our prediction for the dependence of current on distance differs markedly from those based on calculations which implicitly assume energy independent hopping not taking into account the full 3D nature of the problem. In general, our formalism provides a method to compute transport properties through extended NS interfaces with arbitrary hole and barrier shape within the tunneling regime.

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Superconducting flux qubits

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The superconducting flux quantum bit consists of a closed ring with Josephson junctions, biased at about half a magnetic flux quantum through the loop. The two quantum states have opposite circulating current. Previously, quantum superpositions of these two macroscopic states were demonstrated in Stony Brook (single junction loop) and Delft (three junctions). Recently, we succeeded in demonstrating coherent quantum oscillations driven by microwave pulses. Hundreds of oscillations could be induced. Also, simple two- and three-pulse sequences were successfully applied.

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Operation of a two-port charge-phase quantum bit circuit

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We will describe the operation of the "quantronium", a quantum bit circuit [1-2] based on the Cooper pair box. In this new circuit, the box Josephson junction is split into two, thus forming a superconducting loop. The advantage of this design is twofold. First, it provides two separate ports for qubit manipulation and readout. Secondly, it efficiently decouples the qubit from its external environment when the readout is off.

The qubit state is manipulated via pulses applied to the ports. The state is read by measuring the loop current, which is different for both qubit states. This measurement is performed by monitoring the phase response to a current pulse of an ancillary large Josephson junction inserted in the loop.

We demonstrate that all qubit manipulations can be performed by proper combination of dc current pulses on the loop and resonant microwave pulses applied to the charge gate. Using a two-pulse sequence analogous to the Ramsey sequence in atomic physics, we have measured the coherence time. We have also performed echo experiments that show that at least part of the decoherence is caused by low frequency fluctuations of the control parameters.

At the optimal working point, the coherence time corresponds to about 8000 periods of the qubit transition. This time is sufficiently long to envision coupled qubit circuits.

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Electron spin qubits in quantum dots

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We report progress towards the realization of a small-scale quantum computer based on electron spins in lateral GaAs/AlGaAs quantum dots. Starting from the proposal of Loss and DiVincenzo [1], we have developed a set of concrete ideas for initialization, manipulation and read-out of single and coupled spins [2]. We have then realized a few-electron double quantum dot with an integrated charge detector (a QPC). Next, we characterized the energy spectrum of this system and used DC pulses to estimate energy relaxation times. Demonstration of single-shot read-out, electron spin resonance and the SWAP gate are in preparation.

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Decoherence in a Cooper pair shuttle

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We examine [1] decoherence effects in the Josephson current of a Cooper pair shuttle [2], and show that dephasing due to gate voltage fluctuations can either suppress or enhance the critical current and also change its sign. The current noise spectrum displays a peak at the Josephson coupling energy and shows a phase dependence. Finally, we propose an implementation of the shuttle mechanism with a device requiring no mechanically moving part.

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Quasi-particle ballistic transport in hybrid (and other) nanostructures

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Semiconductor nanostructures in appropriate configurations can "host" quasiparticles whose dynamics can be tailored to offer exciting research opportunities both for the study of exotic states and for the implementation of novel device concepts.

I shall present results for the case of ballistic transport in superconductor-semiconductor hybrid systems with the demonstration of de Gennes-Saint James resonant transport in a Nb-GaAs /AlGaAs device. In this context of hybrid systems, the potential of ferromagnet-superconductor junctions for electron microrefridgerators will also be discussed.

Quasiparticles dynamics can be studied also in all-semiconductor nanostructures in the quantum Hall regime. I shall present recent results on non-linear quasiparticle tunneling between fractional quantum Hall edges and discuss them within available theories for the weak-backscattering regime.

Work in collaboration with: F. Giazotto, S. Roddaro, V. Pellegrini, F. Taddei, R. Fazio.

F. Giazotto *et al.* Phys. Rev. Lett. **87**, 216808 (2001), Appl. Phys. Lett. **80**, 3784 (2002).
S. Roddaro *et al.* Phys. Rev. Lett. *in press.*

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Section T: Quantum Transport and Noise

Coulomb drag by small momentum transfer between quantum wires

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We demonstrate that in a wide range of temperatures Coulomb drag between two weakly coupled quantum wires is dominated by processes with a small momentum transfer. Such processes contribute to the drag resistivity because the electron dispersion law is not linear. The small momentum transfer contribution scales with temperature as T^2 if the wires are identical, and as T^5 if the wires are different.

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Interaction, transmission distribution and electromagnetic environment

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Transmission of interacting electrons is a fundamental problem of mesoscopic physics. Recently, we were able to deepen our understanding of this problem with surprisingly simple approach that dates back to [1]. This approach is valid for relatively weak electron-electron interaction, which is its clear disadvantage. The advantage is that the electron transport can be trated within the convenient Landauer-Büttiker framework. The effect of interaction is the renormalization of the transmission coeffiecients. We review our results on i. resonant tunneling in Luttiger liquids [2] ii. environmental effect on counting statistics of electron transfer iii. development of Coulomb blockade in higly conductive quantum dots that were obtained with this approach. We have found unexpected similarities between these groups of phenomena. We were able to formulate simple qualitative conclusions.

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Spin - Charge Separation and Localization in One - Dimension Measured Using Momentum Resolved Tunneling

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We have measured the collective excitation spectrum of interacting electrons in one-dimension. The experiment consists of controlling the energy and momentum of electrons tunneling between two clean and closely situated, parallel quantum wires in a GaAs/AlGaAs heterostructure while measuring the resulting conductance. At high electron densities the measured excitation spectrum clearly deviates from the non-interacting spectrum, attesting to the importance of Coulomb interactions. Notable is an observed 30% enhancement of the velocity of the main excitation branch relative to non-interacting electrons with the same density, a parameter determined experimentally. In short wires, 6μm and 2μm long, finite size effects, resulting from breaking of translational invariance, are observed. Spin - charge separation is manifested through Moiré patterns generated from the spin and charge excitation velocities. At low electron densities the system abruptly looses translational invariance and becomes localized. We find that the localization length corresponds to the inter-electron spacing determined by the one-dimensional electron density.

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Andreev-Lifshitz supersolid for a few electrons on small periodic square lattices

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Using a few electrons interacting via a U/r Coulomb repulsion on small two dimensional $L \times L$ square lattices with periodic boundary conditions and nearest neighbor hopping t, we numerically show that there is a new regime for intermediate values of the Coulomb energy to kinetic energy ratio $r_s = UL/(2t\sqrt{\pi N})$, where delocalized electrons co-exist with a localized Wigner molecule. This supports in an ultimate mesoscopic limit a possibility proposed by Andreev and Lifshitz for the thermodynamic limit: a quantum crystal may have delocalized defects without melting, the number of sites of the crystalline array being smaller than the total number of particles.

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Section P: Selected Posters

Shot noise and multiple Andreev reflections in d-wave superconductors

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We present a theoretical analysis of the shot noise in d-wave/d-wave contacts with arbitrary transparency, including the contribution of multiple Andreev reflections. The multiple charge quanta transferred in these processes are revealed as a huge enhancement of the noise-current ratio at low voltages, which survives for all crystal misorientations. We also show how different ingredients like non-magnetic impurities or a magnetic field produce very characteristic hallmarks in the shot noise, which can be used as a further test of the d-wave scenario in superconducting cuprates.

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A scheme for Quantum Information processing using ballistic electron in the quantum Hall regime

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The implementation of qubits in physical systems is usually based on the realization of two-level systems, or pseudo-spin, to code elementary qubits. Application of *temporal* gates on a qubit allows to perform all necessary rotations on the Bloch sphere. This is the case for ions traps and cavity QED systems in atomic physics, for NMR based systems and, in condensed matter, for coupled quantum dots and superconducting Josephson qubits.

Another approach used for photons in quantum optics is to code a binary quantum information with two distinct propagation modes of a photon (for instance the polarization). *Static* quantum

gates such as polarizers, semi-transparent mirrors and phase shifters can be used to realized elementary operations on a qubit. Using the analogy between electron and photons, it has been proposed that the ballistic propagation of quasiparticles in a quantum conductor can be used in a similar way for quantum computation (flying qubits) [1].

Following this scheme, we propose that electrons propagating on the edge states of a 2D electron system in the Quantum Hall regime should provide a clean realization of flying qubits. The qubit $|0\rangle$ is coded by the presence of an electron in the upper edge while the qubit $|1\rangle$ corresponds to an electron on the lower edge. A quantum Point Contact biased at 1/2 transmission realizes the Hadamard gate, while a gate on one edge provides an adjustable phase shifter. Finally the Coulomb interaction of electrons belonging to two disctinct edge pairs is expected to be strong enough to realize a controlled phase shift. We discuss the injection of electrons on the edges as well as suitable combinations of the three elementary quantum gates to entangle two or more quantum bits.

[1] R. Ionicioiu et al., quant-ph/0011051 (2000).

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Sub-Planck Structure, Decoherence, and Many-Body Environments

Andrew Jordan

UC Santa Barbara and University of Geneva

Mark Srednicki

UC Santa Barbara

In a recent letter to Nature, Zurek has argued that unexpected sub-Planck structures in a quantum chaotic system can generically cause a simple quantum system (which is weakly coupled to the chaotic system) to decohere. We argue that this conclusion holds only if the number of degrees of freedom of the chaotic system is large. Our arguments are based on the Berry-Voros ansatz for the structure of energy eigenstates in chaotic systems. This implies that many-body environments may be crucial for the phenomenon of quantum decoherence.

paper reference: quant-ph/0112139

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Noise correlations, entanglement, and Bell inequalities in nanophysics

Thierry Martin

Centre de Physique Theorique, Universite de la Mediterranee

We describe two situations where positive noise correlations can be directly monitored using a transport experiment, either with a superconductor or with a correlated electron system. Bell

inequalities and quantum mechanical non-locality with electrons injected from a superconductor are addressed first. Next, noise correlations will be computed in a carbon nanotube where electrons are injected in the bulk from a STM tip. The first topic is the result of an ongoing collaboration with G. Lesovik and G. Blatter over the years. The unifying theme is that in both branched quantum circuits, entanglement is explicit and can be illustrated via noise correlations. Entanglement can be achieved either for pairs of electrons in the case of superconductor sources connected to Fermi liquid leads, or alternatively for pairs of quasiparticle excitations of the correlated electron fluid.

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Conductance Anomalies and the Extended Anderson Model for Nearly Perfect Quantum Wires

Tomaz Rejec

Department of Theoretical Physics (F1),
Jozef Stefan Institute, Ljubljana, Slovenia

Anomalies near the conductance threshold of nearly perfect semiconductor quantum wires are explained in terms of singlet and triplet resonances of conduction electrons with a single weaklybound electron in the wire. This is shown to be a universal effect for a wide range of situations in which the effective single-electron confinement is weak. The robustness of this generic behavior is investigated numerically for a wide range of shapes and sizes of cylindrical wires with a bulge. The dependence on gate voltage, source-drain voltage and magnetic field is discussed within the framework of an extended Hubbard model. This model is mapped onto an extended Anderson model, which in the limit of low temperatures is expected to lead to Kondo resonance physics and pronounced many-body effects.

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Measuring the Fano factor of quasiparticles without d.c. bias using photon-assisted shot noise in a Quantum Point Contact

L.-H. Reydellet, P. Roche, and D. C. Glattli

Service de Physique de l'Etat Condensé, CEA Saclay, F-91191 Gif-Sur-Yvette, France

B. Etienne and Y. Jin

Laboratoire de Photonique et de Nanostructures,
CNRS, Route de Nozay, F-91460 Marcoussis, France

We show experimentally that even when no bias voltage is applied to a quantum conductor, the electronic quantum partition noise can be investigated using GHz radiofrequency irradiation of a reservoir. Using a Quantum Point Contact configuration as the ballistic conductor we are

able to make an accurate determination of the partition noise Fano factor resulting from the photon-assisted shot noise. Applying both voltage bias and rf irradiation we are able to make a definitive quantitative test of the scattering theory of photon-assisted shot noise.

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List of Participants

Dr Jan Aarts	University of Leiden
Prof Nicolas Agrait	Universidad Autonoma de Madrid
Mr Mahrous Ahmed	University of Sheffield
Dr James Annett	University of Bristol
Mr James Arnold	UMIST

Mr Stavros Athanasopoulos	Lancaster University
Miss Cecile Bacca	Konstanz University
Dr Adrian Bachtold	Ecole Normale Superieure
Dr Alexi Bagrets	Max-Planck-Institut of Microstructure Physics
Dr Steven Bailey	Lancaster University
Dr Grzegorz Banach	Daresbury Laboratory
Dr Denis Basko	ICTP, Trieste
Prof Vincent Bayot	Universite Catholique de Louvain
Prof Carlo Beenakker	University of Leiden
Dr Joost Bekaert	Leuven
Prof Fabio Beltram	NEST-INFM
Dr Wolfgang Belzig	University of Basel
Prof Stefan Bengtsson	Chalmers University
Dr Jean-Marc Berroir	ENS, LPMC
Prof Peter Beton	Nottingham University
Prof Stefan Blügel	IFF, Forschungszentrum Juelich
Mr Alessandro Braggio	Universita di Genova
Dr Tobias Brandes	UMIST
Prof Arne Brataas	Norwegian University of Science and Technology
Prof Andrew Briggs	Oxford University
Dr Philip Buckle	QinetiQ
Dr Yury Bugoslavsky	Imperial College
Dr Olivier Buisson	CRTBT-CNRS, Grenoble
Dr Bogdan Bulka	Institute of Molecular Physics, Poznan
Dr Doug Burgess	MOD, NX8 Malvern Technology Centre
Prof Markus Buttiker	Universite de Geneve
Mr Anthony Julian Carlick	University of Bristol
Mr Fabio Cavaliere	University of Genova
Prof Venkat Chandrasekhar	Northwestern University
Dr Maxim Chichkine	De Montfort University
Mr Mateusz Cholascinski	Karlsruhe Univeresity
Dr Tord Claeson	Chalmers University of Technology
Dr Fabrizio Cleri	ENEA, Unita Materiali e Nuove Tecnologie
Dr Lesley Cohen	Imperial College
Dr Rolf Crook	University of Cambridge
Mr Michael Croucher	University of Sheffield
Dr Jozsef Cserti	Eotvos University
Prof Per Delsing	Chalmers University of Technology
Dr Ursula Dettlaff	Max Planck Institut for Solid State Research
Dr Rosa Di Felice	Universita di Modena

Dr Paul Dolby	Lancaster University
Dr Janusz Dubowik	Institute of Molecular Physics, Poznan
Prof Eleftherios Economou	IESL-FORTH, Heraklion
Dr Clive Emary	UMIST
Dr Klaus Ensslin	ETH Zurich
Mr Sigurdur Erlingsson	Delft University of Technology
Dr Mattias Eschrig	University of Karlsruhe
Prof Spiros Evangelou	University of Ioannina
Dr Ferdinand Evers	Forschungszentrum Karlsruhe
Dr Giorgos Fagas	Universität Regensberg
Dr Giancarlo Faini	LPN - CNRS, Marcoussis
Prof Giuseppe Falci	Scuola Normal Superiore, Pisa
Prof Volodya Falko	Lancaster University
Mr Peter Falloon	University of Western Australia
Prof Rosario Fazio	Scuola Normal Superiore, Pisa
Dr Mike Fearn	QinetiQ
Dr Denis Feinberg	CNRS, Grenoble
Prof Jaime Ferrer	University of Oviedo
Prof Albert Fert	Universite Paris-Sud
Prof Mike Finnis	Queen's University Belfast
Dr Mikael Fogelstrom	Chalmers University
Dr Christopher Ford	University of Cambridge
Dr Bryan Gallagher	Nottingham University
Dr F Galli	Leiden University
Dr John Gallop	National Physical Laboratory, Middlesex
Prof Gillian Gehring	University of Sheffield
Prof Andrey Geim	University of Manchester
Dr Ulf Gennser	CNRS, Marcoussis
Dr Christian Glattli	CEA Saclay/ENS Paris
Prof Leonid Glazman	University of Minnesota
Dr Guido Goldoni	Universita di Modena e Reggio Emilia
Mr Ian Grace	Lancaster University
Mr Mattias Graeber	University of Basel
Mr Jochen Grebing	University of Constance
Dr Irina Grigorieva	Univeristy of Manchester
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Dr Sanju Gupta	University of Cambridge
Dr Victor Gurarie	Oxford University
Mr Cedric Gustin	Leuven

Prof Pertti Hakonen	Helsinki University of Technology
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Prof David Haviland	Royal Institute of Technology, Stockholm
Prof Frank Hekking	CNRS, Grenoble
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Dr Tarnjit Johal	Daresbury Laboratory
Dr Mats Jonson	Chalmers
Dr Andrew Jordan	Universite de Geneve
Mr Oleg Jouravlev	TU Delft
Prof Tomas Jungwirth	University of Texas at Austin
Prof Paul Kelly	University of Twente
Dr Stefan Kettemann	University of Hamburg
Dr Jurgen Koenig	Universitat Karlsruhe
Dr Kohler Heinerich	Universidad Autonoma de Madrid
Mr Janos Koltai	Eotvos Lorand University, Budapest
Dr Vladislav Korenivski	Royal Institute of Technology, Stockholm
Mr Andor Kormanyos	Lancaster University/ELTE Hungary
Prof Jorg Kotthaus	CeNS, LMU Munchen
Prof Bernhard Kramer	University of Hamburg
Dr Mariusz Krawiec	University of Bristol
Mr Andrew Kretinin	University of Exeter
Mr Vojko Kunej	University of Konstanz
Dr Stefan Kurth	Free University Berlin
Miss Ioanna Kyriakou	QinetiQ
Prof Colin Lambert	Lancaster University
Mr Neill Lambert	UMIST
Dr Michel Lannoo	CNRS-SPM
Mr Alexandru Lerescu	University of Groningen
Prof Igor Lerner	University of Birmingham
Prof Laurent Levy	LCMI/CNRS, Grenoble
Dr Denis L'Hote	CEA Saclay
Mr Gunther Lientschnig	TU Delft
Dr Poul Lindelof	Niels Bohr Institute
Dr Rosa Lopez	Universite de Geneve
Prof Daniel Loss	University of Basel
Dr Procolo Lucignano	Universita' Frederico II Napoli
Dr Massimo Macucci	Pisa
Prof Allan MacDonald	University of Texas at Austin
Dr Dominique Mailly	CNRS Marcoussis

Dr Yuriy Makhlin	University of Karlsruhe
Prof Charles Marcus	Harvard
Dr Miguel Marques	Donostia International Physics Center
Dr Christopher Marrows	University of Leeds
Prof Thierry Martin	Universite de la Mediterranee
Dr Jan Martinek	Universitat Karlsruhe
Mr Riccardo Mazzarello	Universitaet Hamburg
Dr Phil Meeson	University of Bristol
Prof Ingrid Mertig	Martin Luther Universität Halle
Dr Edward McCann	Lancaster University
Prof Laurens Molenkamp	Würzburg University
Dr Rafael Molina	Strasbourg
Dr Elisa Molinari	Modena
Dr Raymond Monk	European Commission
Prof Gilles Montambaux	Universite Paris-Sud
Mr Malachy Montgomery	Queen's University of Belfast
Prof Johan Mooij	Delft University of Technology
Dr Boris Muzykantskii	University of Warwick
Prof Iouli Nazarov	Delft University of Technology
Mr Zoltan Adam Nemeth	CEA, Saclay
Mr Chris Newman	Lancaster University
Dr Jane Nicholson	EPSRC
Mr Konstantin Novoselov	University of Manchester
Dr Andreas Osterloh	Universita di Catania
Dr Bernard Pannetier	CNRS, Grenoble
Mr Neil Pattinson	Lancaster University
Mr Fabian Pauly	University of Karlsruhe
Dr Natalie Pavlenko	Technical University of Munich
Prof Francois Peeters	University of Antwerp
Prof Victor Petrashov	Royal Holloway, University of London
Prof Jean-Louis Pichard	CEA-Saclay
Dr Fabio Pistolesi	CNRS Grenoble
Dr Gloria Platero	Material Science Institute of Madrid
Mr Peter Polinak	Lancaster University
Dr Peter Pollner	ELTE, Budapest
Ms Marta Prada	University of Leeds
Prof Martti Puska	Helsinki University of Technology
Dr Roberto Raimondi	University of Roma Tre
Prof Anton Ramsak	University of Ljubljana
Mr Esa Rasanen	Helsinki University of Technology
Mr Tomaz Rejec	Jozef Stefan Institute, Ljubljana
Prof Klaus Richter	University of Regensburg
Dr Jorge Ripoll	Iesl-Forth

Mr John Robinson	Lancaster University
Mr Alexandre Reily Rocha	Trinity College Dublin
Dr Patrice Roche	CEA, L'orme des Merisiers
Dr Alexandre Roussanov	Leiden University
Dr Sergiy Rozhko	Cambridge Magnetic Refrigeration Ltd
Dr Carlo Rozzi	Freie University of Berlin
Dr Sergey Safonov	University of Exeter
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Dr Peter Samuelsson	Universite de Geneve
Dr David Sanchez	Universite de Geneve
Dr Marc Sanquer	CEA-Grenoble
Dr Stefano Sanvito	Trinity College Dublin
Prof Maura Sassetti	Universita di Genova
Prof Alex Savchenko	University of Exeter
Prof Christian Schonenberger	University of Basel
Dr Ursula Schroeter	University of Constance
Dr Thomas Schulthess	Oak Ridge National Laboratory
Prof Robert Shekhter	Chalmers University
Dr Andrew Shields	Toshiba Research Europe Ltd
Prof Uri Sivan	Technion-Israel
Prof Maurice Skolnick	University of Sheffield
Prof Fernando Sols	Universidad Autonoma de Madrid
Mr James Stanley	Lancaster University
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Prof Hideaki Takayanagi	NTT Basic Research Laboratories
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Dr Grigory Tkachov	Lancaster University
Miss Milica Todorovic	Oxford University
Prof David Tomanek	Michigan State University
Dr Jakub Tworzydlo	Leiden University
Dr Alexander Tzalenchuk	NPL
Dr Cristian Urbina	CEA-CNRS Saclay
Prof Gerrit Van Der Laan	Daresbury Laboratory
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Prof Goran Wendin	Chalmers University of Technology
Dr Robert Whitney	University of Oxford
Mr Laurens Willems van Beveren	TU Delft
Dr David Williams	Hitachi Cambridge Laboratory
Dr Ludger Wirtz	Donostia International Physics Center
Dr Jerzy Wrobel	Polish Academy of Sciences Warszawa
Dr Amir Yacoby	Weizmann Institute for Science
Ms Angelica Zacarias	Free University Berlin
Mr Michele Zaffalon	University of Groningen
Dr Nikolai Zhitenev	Bell Labs, Lucent Technologies
Dr Xenophon Zotos	IRRMA EPFL-PPH Lausanne

3.1.2 Report on the Workshop Framework Programme 6

Paris, January 25, 2003

The Network orgainised a one-day Workshop in Paris to discuss a proposal for a new Marie Curie Research Training Network within the Framework 6. The Agenda of the meeting and the list of participants are attached. As the result of the meeting it was decided to submit a proposal for a Marie Curie RT-Network with the title

Nanospintronics from First Principles

- From new materials to novel phenomena and design concepts.

The proposal will consist of about ten flagship projects centered around new materials and novel phenomena and design concepts for spinelectronics. As special Network activities a series of Workshops, Summerschools and Tutorial Courses is planned. The participants elected Walter Temmerman as Coordinator, Peter Dederichs as Chairman and in addition Ingrid Mertig as Coordinator for Training.

The node structure of the Network will basically not be changed. As new partner the Network welcomed Tomasz Dietl, who heads a new Polish node with participants from Warschau and Poznan. The Network also welcomed the participation, on a financially neutral basis, of an US-node, lead by Peter Levy from New York, and a Japan-node, lead by Hiroshi Katayama-Yoshida from Osaka. Without doubt, all three nodes will strongly strengthen the new Network.

Due to unfortunate circumstances the meeting had to take place in the apartment of Chuck Sommers, which gave the meeting a very friendly and personal atmosphere. We thank Chuck and in particular his wife for their great hospitality.

Peter H. Dederichs

AGENDA

Workshop FP6

1. Welcome and some info about Framework 6.
2. Election of Coordinator, Chairman and Coordinator for Training
3. Discussion of the scientific project including:

- selection of flagship projects
- formulation of milestones and tasks
- the nodes of the Network

— lunch, prepared by Mrs. Sommers —

4. Discussion of the training program including:
   - discussion of special training activities at the host institutions and within the Network
   - workshop topics and organisers
   - 4 Annual Meetings and organisers
   - summer schools and organisers
   - tutorial courses and organisers

— end at about 18:00 —-

List of Participants

FR: Albert Fert, Frederic Petroff, Chuck Sommers (all of Orsay)
Mubarek Alouani (Strasbourg)
DE1: Peter Dederichs (Juelich)
DE2: Patrick Bruno, Ingrid Mertig (Halle)
UK: Walter Temmerman (Daresbury)
James Annett, Balazs Gyorffy (Bristol)
NL: Paul Kelly (Twente)
SE: Susanne Mirbt (Uppsala)
HU: Janos Kollar, Lazlo Szunyogh (Budapest)
AU: Peter Weinberger (Vienna)
CZ: Ilja Turek (Brno)
PL: Tomasz Dietl (Warschau)
USA: Peter Levy (New York)
JAP: Hiroshi Katayama-Yoshida (Osaka)

3.2 RTN1 Workshop Announcements

3.2.1 Joint Workshop on "Spin Mesoscopics"

University of Twente
15-18 March, 2003

Sponsored by

EU RTN "Computational Magnetoelectronics"
NEDO "NanoMagnetoElectronics" network
ESF Working Group "Magneto-Electronics"

With ESF support for the new Psi-k proposal http://psi-k.dl.ac.uk/proposal/ now nearly certain, we will obtain ESF/Psik support for the workshop on "Spin Mesoscopics" at the University of Twente

http://www.tn.utwente.nl/cms/ws2003

from 15-18 March 2003.

This means that it will be possible to provide support - workshop fee and hotel accomodation - for Psik members who are not members of the "Computational Magnetoelectronics" Network to attend the workshop. Because of this recent development, the **deadline for registration will be extended**. Support will be given on a "first come, first served" basis until the ESF subsidy is exhausted.

Participants should reserve their own accomodation. For more details, see the website.

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Computational Materials Science
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The Netherlands

Tel: +31-53-489-3166
Fax: +31-53-489-2910
http://www.tn.utwente.nl/cms

3.2.2 Summer School on New Magnetics

September 15-19, 2003

Bedlewo near Poznań, Poland

Organizers:

Andrzej Jezierski, Andrzej Kowalczyk
Institute of Molecular Physics, PAS, Poznań, Poland
and

Stefan Bluegel
Institut Fuer Festkoerperforchung (IFF) Forschungszentrum, Juelich, Germany

Sponsored by: Centre of Excellence (MMMFE), ESF Psi-k Programme and RT-Network "Computational Magnetoelectronics"

The School is thought to be an international forum for presentation and discussion of novel scientific ideas and experimental results of new magnetic materials. The programme of school will cover the following topics: ***magnetism of correlated electron systems (beyond LDA), multilayers, nanostructures, low-dimensional magnetic systems, magnetic semiconductors, half-metallic systems, f-electron systems, surface magnetism, magnetic anisotropy, non-collinear magnetism, magnetoelectronics, transport in nanostructures, new development in electron spectroscopy and application of a new magnetic materials for future electronics.***

The main objective of the School is to bring together scientists from the Western, Central and Eastern European countries involved in research and application of novel magnetic materials.

The programme of the School is planned to consist of plenary and contributed talks as well as poster presentations. The proceedings including plenary talks and selected contributed papers will be published at the end of 2003.

Total cost of the School is 350 EUR and 250 EUR (reduced fee for students, postdocs and accompanying persons). The fee covers accommodation in hotel, meals and proceedings.

Timetable

1st April 2003 abstract submission and registration deadline.

1st May 2003 notification about acceptance of the abstract.

10th May 2003 deadline for payment of fee.

15th June 2003 deadline for paper.

For details and registration please see the web site

http://www.ifmpan.poznan.pl/mmmfe/nm.html

e-mail: nm03@ifmpan.poznan.pl

3.2.3 International Workshop on Diluted Magnetic Semiconductors

June 12-14, 2003

at CECAM, Lyon, France

Sponsors:
RT Network "Computational Magnetoelectronics"
ESF Programme "Towards Atomistic Materials Design (Psi-k)"
Centre Européen de Calcul Atomique and Moléculaire (CECAM), Lyon

Organisers:
Peter H. Dederichs, Research Center Jülich, Jülich (p.h.dederichs@fz-juelich.de)
Josef Kudrnovský, Academy of Sciences, Prague (kudrnovsky@fzu.cz)
Allan H. MacDonald, University of Texas at Austin, Austin (macd@physics.utexas.edu)

Scope:
The workshop aims at a deeper understanding of diluted magnetic semiconductors and brings together theorists from the ab-initio and model Hamiltonian field with leading experimentalists.

The programme will consist of 10 longer reviews, 15-20 shorter talks and a poster session. The attendance will be limited to about 40 participants. More information will be circulated soon.

Deadlines:
Registration: April 1, 2003
Abstracts: April 30, 2003

4 News from the RTN2

"Ab initio Computation of Electronic Properties of f-electron Materials"

4.1 RTN2 Position Announcements

RTN POSTDOCTORAL POSITION IN THE FIELD OF DYNAMICAL MEAN-FIELD THEORY AND ELECTRONIC STRUCTURE CALCULATIONS

(Paris, France)

Applications are invited for a postdoctoral position in the field of Electronic Structure Calculations for Strongly Correlated Materials, and in particular the application and development of Dynamical Mean-Field Theory in the context of electronic structure calculations.

The position, to begin September 2003, is in the context of the European Research and Training Network (RTN) on "Ab initio Computation of Electronic Properties of f-electron Materials". Candidates must be nationals of a MEMBER STATE of the EU or of an ASSOCIATED STATE, and must NOT be citizens of France nor have resided or worked in this country for more than 18 of the 24 months prior to employment.

The applicants should have a solid background in solid-state theory, and preferably some experience in electronic structure calculations and codes (DFT-LDA or GW) and/or many-body theory, as well as appropriate computer skills.

Applicants must send (i) a curriculum vitae, (ii) a list of publications, (iii) a summary of current and proposed research, and (iv) a list of three references with phone numbers and emails, to:

Antoine Georges
Laboratoire de Physique Theorique
Ecole Normale Superieure
24 rue Lhomond
75231 Paris Cedex 05
France

or electronically to:

georges@lpt.ens.fr

Reviewing of applications will start immediately, but the position will be kept open until filled.

5 News from the ESF Programme

"Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces"

5.1 Chairman's Annual Report for 2002

This is the final year of the Programme and again there has been a strong continuation and development of the activities.

The following figures include the planned activities to the end of the current financial year.

This year there are seven research workshops covering a wide range of topics from the Diffusion Quantum Monte Carlo method to hybrid interfaces between ferromagnets and superconductors or semiconductors for nanotechnology. One workshop on 'Catalysis from First Principles' specifically involves active participations of scientists in industry. Three more workshops focussed on joint development of computer codes for our comunity which is a new emphasis. Two of the workshops were organised jointly with CECAM with whom we have growing links as noted in last year's report.

The methodology of ab initio computer simulation is very very sophisticated with many strands and tricks and cross connections. The training of young researchers is therefore very important, and even the strongest groups find that their PhD students benefit from attending specific Summer Schools of which 3 received partial funding from the Programme. Equally important are the three 'hands-on' tutorials usually running for a week, which provide training in the use of a particular code including background theory. Symposia in our field have been organised at 3 conferences, which provide an important link with experimentalists. One of the features of some modern experimental tools is that the measured data cannot be interpreted fully or uniquely without accompanying computer simulations, something that is of growing importance in our field.

The association of our community with the EURESCO conferences continues, and we have had again to contribute financially to 'our' conference in the series now entitled 'Electronic Structure of Solids and Other Systems'. This year the topic was 'Biophysics from First Principles: From the Electronic to the Mesoscale', and this has initiated a new series on 'Computational Biophysics: Integrating Theoretical Physics and Biology'.

However, serious consideration is being given to working in future with the Gordon conference organisation in Europe, because it is so much more consistent and satisfactory to deal with than EURESCO.

As this is the final year of the ESF STRUC Programme, much effort since last October has gone into working for the survival of our communal activities. As our community did not go through the stage of an ESF Network but proceeded directly to an ESF Programme, the ESF has allowed us to submit a new Programme proposal to start in 2003, for which we are extremely grateful. That proposal was selected by ESF and is now under consideration by ESF Member Organisation for joining and funding.

Looking even further ahead, we note that the EU has broadened somewhat its ideas on infrastructures, and making a proposal in that direction is being considered. It is clear to us, even if not to the EU, that the networking and collaborative code development organised through the ESF Psi-k (STRUC) and SIMU Programmes provide the software and expertise infrastructure that our research community needs on a long term basis.

Volker Heine, chairman

Cambridge, 6 October 2002

5.2 Minutes of the Steering Group

Paris, 12 October 2002

Present

Volker Heine	Chair, Cavendish Laboratory, Cambridge, UK
Igor Abrikosov	Uppsala University, Sweden
Geert Brocks	Twente University, NL (replacing Paul Kelly)
Stefan Bluegel	Osnabrück University, Germany
Stefaan Cottenier	KU Leuven, Belgium
Peter Dederichs	KFZ Juelich, Germany
Hugues Dreyssé	Université L. Pasteur, Strasbourg, France
Claudia Filippi	Leiden University, Netherlands
Mike Finnis	Queens University, Belfast, United Kingdom
Xavier Gonze	Université Catholique de Louvain, Belgium
Eberhard K.U. Gross	Freie Universität Berlin, Germany
Jürgen Hafner	Vienna University, Austria
Adam Kiejna	Wroclaw University, Poland
Tone Kokalj	Stefan Institute, Ljubljana, Slovenia
Janos Kollar	Res Inst. F. Solid State Phys, Budapest, HU
Jose Luis Martins	INESC, Lisboa, Portugal
René Monnier	ETH Hönggerberg, Zurich, Switzerland
Risto Nieminen	Helsinki University of Technology, Finland
Pablo Ordejon	Inst. De Materials, Barcelona, Spain
Hariton Polatoglou	Aristotle University, Thessaloniki, Greece
Charles H. Patterson	Trinity College, Dublin, Ireland
Raffaele Resta	SISSA, Trieste, Italy
Angel Rubio	Univ. Pais Vasco, San Sebastian, Spain
Axel Svane	Universität Aarhus, Denmark
Z. (Dzidka) Szotek	Daresbury Laboratory, United Kingdom
Walter M. Temmerman	Daresbury Labortory, Secretary, UK
Ilja Turek	Inst. Phys. Materials, Brno, Czech Republic
Catherine Werner	ESF Administrator

Apologies

Ole Krogh Andersen	MPI FKF, Stuttgart, Germany
Paolo Carloni	SISSA, Trieste, Italy
Alessandro de Vita	Univ. Trieste and EPFL Lausanne
Christian Elsaesser	MPI Metallforschung, Stuttgart, Germany
Antoine Georges	Ecole Normale Supérieure, Paris, France
Matthias Scheffler	MPI Fritz Haber Institute, Berlin, Germany

0. **Welcome and introduction**

Professor V. Heine opened the meeting and welcomed everybody. He explained that this meeting was a combination of two events: the fifth and last meeting of the Core Steering Group of the STRUC Ψ_k programme and a workshop inviting all members involved in the new programme "Towards Atomistic Materials Design" (potential members of the steering committee and spokesperson of the 15 working groups). This new programme was approved by the ESF Standing Committee for Physical and Engineering Sciences (PESC) and will be officially launched in January 2003 providing that sufficient funding has been secured from Member Organisations.

1. **Approval of the minutes of the last meeting**

The minutes of the last meeting of the Core Steering Group (Paris, 6 October 2001) were approved without changes.

2. **Matters arising from the minutes since the last meeting**

Several events did not take place in 2002 as planned and will be postponed to the first months of 2003.

2.1. "Hybrid Interfaces". This 3 day workshop, organised by W.M. Temmerman, will be shifted to 5 January 2003. It will be attached to the end of the International Conference on Nanoelectronics which will take place in Lancaster on 6-10 January 2003. (Budget 9,000 EUR)

2.2. Hands-on tutorial course on the VASP code. This course, organised by J. Hafner, will be delayed until February 2003 because of an insufficient number of working places and pending work on a GUI for VASP.(Budget: 10,000 EUR)

2.4. S. Bluegel's tutorial on LAPW, which had been postponed several times, will now take place as "LAPW developers miniworkshop" on 10-11 February 2003. (Budget: 4,000 EUR).

2.3. First International ABINIT Developer Workshop. This workshop, organised by Xavier Gonze, will take place on 6-8 November 2002 in Louvain-la-Neuve. Members had been informed by e-mail of the programmes support for this workshop (Budget: 2,100 EUR).

3. **Financial situation**

All these events will be financed from the unspent balance of the programme at the end of 2002. Should there still be some money left after having financed all these workshops, members agreed that an extra payment of 20,000 EUR (4,000 EUR x 5 years) should be made as a contribution to Z. Szotek's work for the programme's Newsletter. C. Werner informed the Committee that all claims for expenses should reach the ESF before the end of March 2003, when the Programme's accounts will be closed.

4. **Chairman's report on 2002**

The Chairman's report for the year 2002 had been circulated to the members. V. Heine commented that the programme had been very active in 2002 supporting altogether 7 workshops, 3 summer schools, 3 hands-on tutorials, 3 conferences/symposia, one EURESCO conference and one visit. Detailed reports on all visits and workshops which took place during the year 2002 appear in the Ψ_k Newsletter. The Chairman also informed the Committee that the proposal for a EURESCO Conference for 2003, submitted by W. Temmerman and A. Georges and supported by M. Scheffler and V. Heine, had been turned down by the ESF office.

The Chairman closed this part of the meeting by thanking W. Temmerman, Z. Szotek and C. Werner for their work in the running of the programme.

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5. V. Heine explained that he had invited to this large meeting all members listed as potential members of the Steering Committee of the new programme and the spokespersons of the 15 working groups listed in the programme's proposal. He informed the participants that the referees' reports on the programme proposal were very good and that the proposal had now been sent to ESF Member Organisations with an "invitation" for financial support. So far, positive replies have been received from: Austria, Belgium (Flanders), Finland, Italy, Netherlands, Spain and Sweden. He invited the members whose Member Organisations had not yet replied to do some lobbying, if possible.

Since the programme is not yet officially launched and has not secured its funding, it should be understood that the decisions and commitments for support of activities cannot be considered as firm and will have to be ratified in early 2003, possibly by e-mail.

The new programme will have as interim chairman, Volker Heine, until March 2004 when Peter Dederichs will take over this position. It is organised around 15 working groups:

Working Groups on "Ab initio quantum many-body calculations on real materials". [Walter Temmerman (UK) Coordinator and Spokesperson for methods not included below]

WG1: GW method [A. Rubio (Spain)]
WG2: Quantum Monte Carlo method (QMC) [Claudia Filippi (NL)]
WG3: Dynamical Mean Field Theory (DMFT) [A. Georges (France)]

Working Groups on "Tackling larger systems"

WG4: Linear scaling and local orbitals [P. Ordejon (Spain)]
WG5: Hybrid quantum and classical methods [A.DeVita(Switzerland and Italy)]
WG6: Catalysis and surface science [J. Hafner (Austria)]

Working Groups on "Semiconducting electronics"

WG7: Semiconductors and nanotechnology [R. Nieminen (Finland)]
WG8: Electronics at the molecular level [group just being formed]

Working Groups on "Magnetism" [P. Dederichs (Germany) Coordinator]

WG9: Magneto-electronics [P. Kelly (Netherlands)]
WG10: f-electron systems [A. Svane (Denmark)]
WG11: Complex magnetism and nanostructures [S. Bluegel (Germany)]
WG12: Ab initio simulations for biology [P. Carloni (Italy)]
WG13: Minerals and related materials [S. Scandolo (Italy)]
WG14: Grain boundaries and interfaces [C. Elsaeser (Germany)]
WG15: Ab initio design of structural materials [I. Abrikosov (Sweden)]

It was mentioned that the system of working groups under the old STRUC Ψ_k programme did not work satisfactorily; maybe because their role had not been clearly defined and the spokespersons had no occasion to meet and report. Members agreed that with the new programme, the spokespersons should meet once a year, on the occasion of the steering committee meeting.

6. Members also thought that an effort should be made to have closer links with industry and demonstrate the programme's willingness to co-operate with industry since 8 out of the 15 working groups have an "industrial application flavour" including even WG12 on biology and biological systems. However, previous experience shows that it is rather difficult to work with them since there will always be the problem of industry not wanting to reveal secrets. But industry should inform scientists about their needs and which field should be developed as a whole.

J. Hafner referred to the success of the special workshop with people from industry held at the beginning of the old Ψ_k programme, which has resulted in a continuous series of joint workshops on Catalysis from First Principles. It is time to try again with other industries and Hafner offered to try to arrange a similar workshop in 2003 or 2004.

It was also suggested to write articles for journals more linked to industry.

7. European Materials Research Society (EMRS). Members agreed that the programme should increase its visibility in these meetings. The EMRS programme for 2003 has already been finalised but suggestions could be made for 2004. The Ψ_k programme should hold focussed

meetings attractive to industry. H. Dreyss is still ready to act as the link with EMRS.

8. Psi-k 2005 Conference. This Conference organised by R. Nieminen will take place in Schwaebisch Gmuend following the same format as the two previous big conferences and involving the working groups.

9. Newsletter. Dzidka Szotek reported on this item. With a distribution list of more than 1,000 names, the Ψ_k Newsletter reaches a large audience and is considered as a very useful tool by the scientists. However, Dzidka Szotek invited once again suggestions for scientific highlights and new initiatives. She also commented that the section on abstracts seemed to be declining. She suggested that group leaders collect the abstracts in their groups and submit them to the Newsletter. She reminded everybody that these abstracts must be written in latex and use the templates available on the web site. Members also commented that if the Newsletter was to be useful, the whole community should submit abstracts.

10. Integrated Infrastructure Initiative (I3)

V. Heine reported on this issue. It is a programme of the European Commission to support research infrastructure in Europe. The EC has now opened the funding to "virtual" centres and software infrastructure. In this context, a proposal entitled "Atomic-Scale Computer Simulations of Materials Across Many Sciences" will be written in collaboration with W. Temmerman, M. Mareschal (chairman of the ESF-SIMU programme) and P. Durham. A meeting on this I3 initiative took place on 11 October 2002 and the proposal will be submitted to the EC after the call has been issued. The idea of this programme is to bring together all groups involved in developing large codes and to get funding for the developments and compatibility of these codes, as well as providing for workshops and other networking activities, on hopefully a longer term basis than is possible under the ESF Psi-k and SIMU Programmes. Nine leading centres have been contacted, CECAM being one of them and envisaged as the management centre.

11. **Outline budget for 2003**

The new Ψ_k Programme asked for a budget of 185,000 EUR. If the totality of the funds could be secured, the breakdown of this "optimistic" budget would be the following:

17 kEUR for annual committee meetings and review of working groups
16 kEUR for the Newsletter
9.3 kEUR for ESF administrative costs
5 kEUR for individual visits
20 kEUR set aside for the psi-k 2005 conference
117 kEUR for workshops, tutorials and summerschools

Any shortfall in the total contributed by the ESF Member Organisations would have to be taken out of the allocation for workshops, etc..

12. **Support to workshops, tutorials and conferences**

Twenty proposals for workshops, tutorials and conferences had been received and were discussed during the meeting. No formal decisions could be taken at the time of the meeting since the programme had no legal existence yet. It will be officially launched in January 2003 when the budget will also be known. Decisions will then have to be adjusted accordingly and/or ratified by e-mail in early 2003.

12.1 *Ab-initio understanding of superconducting and normal state properties of MgB2.* Organisers: Ole K. Andersen, Jens Kortus, Giovanni B. Bachelet, Luciano Pietronero. This workshop, gathering 20 invited speakers with a mix of theory and related experiment and 30 young scientists, would take place at Rome University on 2-4 July 2003. Members decided to allocate 7 kEUR for this workshop.

12.2 *Application of Density-Functional Theory in Condensed-Matter Physics, Surface Physics, Chemistry, Engineering and Biology.* Organisers: Catherine Stampfl, Joerg Neugebauer, Peter Kratzer, Arno Schindlmayr and Matthias Scheffler. This hands-on tutorial will take place at the Fritz Haber Institut in Berlin on 21-30 July 2003 with a maximum number of 70 participants. 13KEUR were allocated.

12.3 *XVII International Winterschool on Electronic Properties of Novel Materials.* Organisers: Hans Kuzmany, Siegmar Roth, Joerg Fink and Michael Mehring. It will be organised in Kirchberg in Austria on 8-15 March 2003. No support was granted for this winter school.

12.4 *Ab-Initio Electron-Excitations Theory: Towards Systems of Biological Interest.* Organisers: Pablo Garcia-Gonzalez, Maurizia Paulummo, Olivia Pulci, Arno Schindlmayr, Nathalie Vast. This 4-day workshop would be held at DIPC in San Sebastian, Spain on 21-24 September 2003 involving Working Group 1. It was decided to support this workshop with the sum of 7 kEUR.

12.5 *Software solutions for data exchange and codegluing.* Organisers: X. Gonze and K. Hinsen. This 3 day workshop has asked to be co-sponsored by CECAM and the SIMU programme. It would take place at CECAM in Lyon. The sum of 4 kEUR was allocated.

12.6 *Recent advances in the theory of nanotubes.* Organisers: Oguz Gulseren, Marco Nardelli, Angel Rubio. This is a joint workshop application to Psi-k and CECAM which will take place in summer 2003. A support of 3kEUR was granted.

12.7 *Spin Mesoscopics.* Organisers: Paul J. Kelly and E.W. Bauer. This workshop planned for 15-18 March 2003 (University of Twente) would be an opportunity for Working Group 9 to get together. Members decided to allocate a sum of 7 kEUR for this event.

12.8 *XIII workshop on Computational Materials Science.* Organisers: V. Fiorentino, F. Bernardini and P. Ruggerone. This workshop, which is more or less a summerschool, will be held in Villasinius, Sardinia. A sum of 7 kEUR was approved with the condition that it helped the participation of PhD students from outside Italy.

12.9 *Reactive classical potentials versus hybrid methods: towards chemical complexity.* Organiser:

Jean-Bernard Maillet. Members thought that the proposal they had in front of them had its weaknesses and questioned the usefulness of holding a second workshop on this topic after the CECAM/SIMU workshop held in July 2002. They decided not to support this initiative, although it involves WG 9.

12.10 *Position operator r in extended systems within DFT and HF.* Organisers: Michael Springborg and Raffaele Resta. This workshop is seeking partial support from CECAM. The Committee decided to allocate 5 kEUR.

12.11 *Electronic Transport in Molecular Systems.* Organisers: Xavier Blase, Christophe Delerue and Kurt Stokbro. This 3-day workshop would be held at CECAM beginning of June 2003.

12.12 *Electronics at the Molecular Level.* Organiser: Risto Nieminen. It would tentatively take place in San Sebastian, Spain on 10-13 February 2003. Members thought that these two workshops 8.11 and 8.12 were important workshops especially as a kick off meeting for working group 8 but since the topics were overlapping, it was decided that only one event could be supported. R. Nieminen will contact the organisers of the other workshop to see how the two events could be merged. 10 KEUR were put aside.

12.13 *Summer School on New Magnetics.* Organisers: Andrzej Jezierski, Andrzej Kowalczyk and Stefan Bluegel. This school is co-sponsored by an EU network and woud be the occasion for Working Group 11 to get together. It will take place in Poznan, Poland. A support of 3 kEUR was approved.

12.14 *Dilute Magnetic Semiconductors.* Organisers: Peter H. Dederichs, Josef Kudrnovsky and Allan H. MacDonald. This workshop involving Working Group 9 will be co-sponsored by the RT-Network "Computational Magnetoelectronics" and has applied also to CECAM. It will be held on 12-14 June 2003 at CECAM. A support of 6 kEUR was allocated.

12.15 *Hands-on training course on VASP.* This workshop was discussed under 2.4 of these minutes and will be financed out of the 2002 budget.

12.16 *Ab-initio many-body for correlated electron systems.* Organisers: Walter Temmerman and Antoine Georges. This 5-day conference will bring together 100 scientists at the ICTP in Trieste on 25-29 August 2003. Members decided to support this conference with the sum of 15 kEUR. This is the same excellent proposal involving WG 3 that was rejected by ESF as a EURESCO Conference and has now found sponsorship from ICTP and other sources.

12.17 *High Performance Computing with the ABINIT Code.* Organisers: Xavier Gonze and P. Ghosez. This would be a second workshop on this topic (after the November 2002 one for which 38 participants had already registered). Members decided a support of 3 kEUR for this workshop which will take place in Paris in 2003 or early 2004.

12.18 *International workshop on solving the Bogoliubov de Gennes (BdG) Equation.* Organisers: Balazs L. Gyorffy and James F. Annett. This VII workshop in a series with the above title will be held at Bristol University on 30 May-1 June 2003. A support of 4 kEUR was approved.

12.19 *Ab-initio design of structural materials.*: Organiser: Igor A. Abrikosov. This would represent the start-up meeting of Working Group 15. 9 kEUR were allocated for this event which

will take place at Uppsala University.

12.20 *Summer School on Linear Scaling with Hands-on Siesta Tutorial.* Organiser: Emilio Artacho. This school is supported by Working Group 4 and and is applying to be co-sponsored by CECAM. It was decided to support this school with the sum of 4kEUR. Volker Heine noted that eight working groups were represented in these proposals for workshops, conferences and schools, namely WGs 1, 3, 4, 5, 8, 9, 11 and 15. He invited the spokespersons of the other working groups to briefly report on their work plans and reminded the members present that the modest budget of the whole programme will only allow two or three workshop per working group over the whole duration of the programme.

12.21 *Workshop with Industry.* Organiser: J. Hafner. We overlooked making any specific allocation for this workshop from Minute 5 above.

13. **Date and place of next meeting**

The next meeting of the Steering Committee including spokespersons of working groups will take place in Paris on 4 October 2003.

5.3 Latest news about the new ESF Psi-k Programme

The funding for our type of ESF Programme follows what the ESF call the a-la-carte principle, namely that each country (to be precise, each research council in each country) can decide for itself whether it wishes to join and contribute financially towards any proposed Programme.

The good news is that enough pledges have now been received from enough countries to guarantee over 80 percent of the budget that we had proposed in our application last year. This is sufficient for the ESF Council and we expect it to launch the new Psi-k Programme at its next meeting on 5-6 February, 2003. Negotiations are still continuing with some countries that have not yet committed themselves but where there are scientists who think that they should join too.

Volker Heine, Chairman

26 January, 2003

5.4 A completely new initiative for our whole community

I want to give some preliminary information about plans being discussed for a proposal to the European Union for an "Integrated Infrastructure Initiative"(I3), which is a new type of scheme in the new Framework Programme FP6. A tentative title is "A Software Infrastructure for Atomic-Scale Computer Simulations of Materials for Many Sciences" with acronym perhaps SIASS. It would cover both ab initio simulation, and the work of our colleagues in the SIMU community based more on statistical mechanics. They are concerned with how to do atomic-scale simulations when there are various difficulties, including long length scales due to elastic interactions, long time scales for activated processes, and navigating in a complicated free-energy landscape such as in protein folding. The simulation may be with a classical interatomic force model or may be ab initio with quantum mechanics, so that our two communities are overlapping increasingly.

I see four factors that are coming together here. Firstly there is the harsh fact that there can be no renewal of our ESF Psi-k Programme after the end of the new Programme in 2007. Those are the rules. ESF has already shown flexibility by allowing us a new (second) application because we did not go through the normal route of having an ESF Network before the first ESF Programme. The same will apply to the SIMU community who have a second application in at the present time. So we need to find another source of funding beside the ESF.

Secondly there is clearly a longer term need. Computer simulation is not going to disappear in 5 years time! Indeed I see active development over the next 20 years, judging by the last 20 years. I note the new developments in treating more strongly correlated electron systems by various means, and the possibility of getting 'chemical accuracy' with Quantum Monte Carlo in more ordinary situations. At the same time there is a rapid growth in the range of applications. So we need some longer term basis of support. I think it is also widely recognised that the excellence of research in our field in Europe has been greatly helped by the excellent networking and collaboration built up over the last 20 years. So we need the longer term basis in order to continue doing first class science.

Thirdly we have recognised that our Psi-k organisation has the role of an infrastructure for our community. There is now a well developed pattern of research workshops, summer schools and training sessions often with hands-on experience of codes, The Psi-k Newsletter, individual visits, a big conference every five years, etc.. Experimentalists often have big machines such as synchrotron or neutron source, whose institutions also act as intellectual centres for 'networking' and spreading best practise. However most of our work is done on in-house computers and even

large computer centres are only accessed electronically. In our community it is the sharing of expertise through Psi-k type of activities, and the use of shared computer codes, that is our necessary infrastructure. Happily the European Union is giving some indication of recognising that there are wider types of infrastructure than the large machines that they like to think of. In discussions which three of us had in Brussels last August, the EU official admitted that our 'software infrastructure' would stretch their ideas on infrastructures to their limits, but he encouraged us to try an application under the I3 scheme. Although a grant would be for 5 years, it would be of a type that can in principle be renewed, and indeed the whole concept of infrastructures is that they continue.

Fourthly the excellence of research in our field in Europe has depended on several excellent computer codes, and the future requires continuous innovation in this direction. However there is a widespread experience that it is very difficult to get financial support for code development from national sources, a point reinforced by a couple of grant refusals recently. Experimentalists have an analogous problem. The I3 scheme has specific provision for such activities, citing as an example building a new instrument which I interpret as a new code in our case. Discussions I have had over the last year have shown there is a tremendous pent-up demand for this, with long lists of capabilities that code users want to have in codes.

Well, I have written at length about the general ides, partly because details are still vague and partly because "There Is No Gain Without Pain!" and some of it has already started. People ask "Why include that and not this?". The pain of dealing with the EU burocratic process is a training for purgatory! Moreover our chaps don't like being 'integrated': I always think there are some physicists who like hunting in large armies and join work in particle physics or astronomy, while condensed matter physics is the last refuge for the individualist.

The plan is to link ('integrate') important centres who are already providing infrastructural services to our community. These will include CECAM, Daresbury, Vienna, Berlin, Copenhagen, Louvain (ABINIT code), Zuerich (Parrinello, Hutter), a new grouping DEMOCRITOS around Trieste in Italy, Barcelona (SIESTA code), Evry (ORAC code on the SIMU side). A few other places will be centres around which some specific code will be developed. The overall coordinator will be Michel Mareschal who has been the chairman of the ESF SIMU Programme and first initiated the idea of an I3. He has recently been reappointed for a further four years as director of CECAM. I think this will strengthen CECAM as an ongoing infrastructure for our community and link it more closely to our scientific community. The plan is for a budget between 1.5 and 2.0 Mega-euros per year, large enough to be of interest to the EU (they like big projects 'to structure the European research community'), but small enough to fit in as a new type of infrastructure between the big spenders like CERN and GRID. Much of the money would go on postdocs for code development. There will also be the type of networking done by Psi-k and SIMU, plus postdoc help for disseminating the use of codes. For example one person told me recently that she has three codes that people want to use, but she has only put one of

them on the web because she could not cope with any more demands for 'support' from users.

What are the chances of success? No-one has any idea, but if we do not succeed this first time, we can fight again in the future. The point is that we deserve to win, and should persevere until we do!

Volker Heine, Psi-k chairman

26 January, 2003

5.5 ESF Programme Workshop Announcements

5.5.1 Start-up Meeting of Work Group 15

Ab initio design of structural materials

February 14-15, 2003

Angstromlaboratoriet, Uppsala, Sweden

A start-up meeting of Work Group 15 "Ab inito design of structural materials"

(http://psi-k.dl.ac.uk/proposal/WG15.htm)

of a new ESF Programme "Towards atomistic materials design" (Psi-k) will take place in Uppsala, Sweden, February 14-15, 2003.

The main question of this workshop is "What is ab initio design of structural materials?" Particular examples of applications of the first-principles electronic theory for the investigations of technological materials and/or problems within materials sciences relevant for the industry will be presented and discussed. Moreover, we will discuss in detail possibilities to combine ab initio calculations with phenomenological schemes, because currently this combination seems to be the most efficient way to solving problems for highly complex technological materials. Speakers are encouraged to spend some time on the issue regarding the usefulness of the obtained results for the customers of their research. They are also encouraged to communicate basic contents of the works so that the audience can pick up ideas for potential joint work. The workshop aims to provide a possibility for discussions between participants regarding future bilateral collaboration and/or teambuilding.

Preliminary list of Invited Speakers include

Antonis N. Andriotis (Greece), Thomas Bligaard (Denmark), Michele Catti (Italy), H. Dreysse (France), H. Ebert (Germany), O. Eriksson (Sweden), Adam Kiejna (Poland), Janos Kollar (Hungary), A. Lichtenstein (The Netherlands), Juan J. Novoa (Spain), Nicolas Papanicolaou (Greece), Krzysztof Parlinski (Poland), Alain Pasturel (France), Anthony T. Paxton (UK), Hariton Polatoglou (Greece), A. V. Ruban (Denmark), S. I. Simak (Sweden), V. S. Stepanyuk (Germany), I. Turek (Czech Republic), Yu.Kh. Vekilov (Russia), Levente Vitos (Hungary), Perla Wahnón (Spain), and Rudolf Zeller (Germany).

Preliminary programme for the workshop can be found at

http://www.fysik4.fysik.uu.se/ (under Events) and

http://psi-k.dl.ac.uk/proposal/WG15.htm.

Uppsala is conveniently located just 30 min. from Stockholm International Airport Arlanda with excellent connections to both, the airport and Stockholm. More information about the Angstromlaboratory can be found at http://www.fysik.uu.se/english/. Limited financial support is available for travel and local expanses. Abstracts (maximum one A4 page, Word or text format) should have been submitted before January 15, 2003 to Igor Abrikosov (Igor.Abrikosov@fysik.uu.se).

5.5.2 Berlin Hands-on Workshop

Application of Density-Functional Theory in Condensed Matter Physics, Surface Physics, Chemistry, Engineering, and Biology

Fritz-Haber-Institut, Berlin

July 21-30, 2003

A hands-on workshop will be held at the Fritz-Haber-Institut, Berlin, Germany, from July 21-30, 2003, organised by the Theory Department. The main objectives of the workshop is to introduce density-functional theory calculations to a level such that the participants obtain a thorough understanding of what DFT can offer and are able to perform such calculations.

Scope of the workshop

The workshop comprises morning lectures by invited experts and afternoon practical exercises at a PC. The lectures will cover the fundamental background of density-functional theory, as well as current developments in time-dependent density-functional theory, the *GW* approximation, novel exchange-correlation functionals, and state-of-the-art applications to physical, chemical, and biological systems. Other first-principles approaches will also be discussed (e.g. FP-LAPW, APW+lo, PAW, and DMol^3).

In the afternoon practical exercises at a PC, the participants will become familiar with the handling of a large program for electronic-structure calculations, whereby they will be able to solve new problems for their own research with this method.

The new plane-wave computer program SFHIngX developed at the Fritz-Haber-Institut will be used for the practical sessions. Participants will receive a free licence of the program for one year.

Participants who have already started a research project in a field related to the workshop topic are encouraged to present their current work in a poster session.

Attendance:

Applications from graduate students working on Ph.D. projects, new post-docs and young, active faculty members are particularly encouraged. A background in quantum mechanics and the physics and chemistry of bonding is required, and experience with personal computers under

Windows or Linux would be helpful.

Instructions on how to apply for the workshop and other information can be found on the web-page:

http://www.fhi-berlin.mpg.de/th/Meetings/FHImd2003/

All application documents should be sent by 15 February 2003.

Inquiries received after 15 February 2003 can only be considered subject to remaining vacancies.

The workshop is sponsored by the Ψ_k-Research Programme *Towards Atomistic Materials Design* of the European Science Foundation. We hope to be able to offer partial support (for local expenses, but not travel) out of these funds to assist participants without other adequate financial support.

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http://www.fhi-berlin.mpg.de/th/Meetings/FHImd2003/

Lectures include	
Monday, 21 July: Introduction	**Friday, 25 July: Ab initio Methods**
M. Scheffler (FHI Berlin)	P. Blaha (Technical Univ. Vienna/Austria)
Present status of ab initio electronic	*The FP-LAPW and APW+lo methods*
structure calculations	P. Bloechl (Technical Univ. Clausthal)
P. Kratzer (FHI Berlin)	*The PAW method*
A fast guide to DFT calculations	B. Delley (Paul Scherrer Inst.)/J.Behler (FHI Berlin)
	DMol^3
	M. Scheffler (FHI Berlin)
	Comparison of first-principles methods
Tuesday, 22 July: Plane Wave Method	**Monday, 28 July: Molecular Dynamics**
E. Pehlke (Technical Univ. Kiel)	J. Neugebauer (FHI Berlin)
The plane-wave pseudopotential method	*Energy barriers, diffusion, kinetics*
M. Fuchs (FHI Berlin)	L. Ismer (FHI Berlin)
Pseudopotentials	*First-principles molecular dynamics*
Wednesday, 23 July: Methodology	**Tuesday, 29 July: Improved band gaps**
J. Neugebauer (FHI Berlin)	S. Kurt/E.K.U. Gross (Freie Univ. Berlin)
Algorithms for total energy minimisation	*Fundamentals of DFT and Time-dependent-DFT*
P. Kratzer (FHI Berlin)	A. Qteish (FHI Berlin/Yarmouk Univ. Irbid-Jordan)
Prerequisites for reliable modelling	*Exact Exchange*
S. Boeck (FHI Berlin)	A. Schindlmayr (Forschungszentrum Juelich)
Introduction to the new plane wave code	*The GW approximation*
Thursday, 24 July, Surfaces	**Wednesday, 30 July, Engineering, Biology**
M. Fuchs (FHI Berlin)	J. Dabrowski (IHP microelectronics, Frankfurt/Oder)
Exchange-correlation energy	*Predictive simulations for microelectronics devices*
E. Pehlke (Technical Univ. Kiel)	J. Ireta (FHI Berlin)
Surface structure, chemisorption, and reactions	*Structural analysis of biological systems*
K. Reuter (FOM Instituut, Amsterdam)	
Ab initio atomistic thermodynamics	

5.5.3 Announcement of a CECAM - Psi-k - SIMU Joint Tutorial

Software solutions for data exchange and code gluing

Lyon, 8-10 october, 2003

Organizers :

X. Gonze, gonze@pcpm.ucl.ac.be

K. Hinsen, hinsen@cnrs-orleans.fr

Purpose:

In this tutorial, we will teach software tools and standards that have recently emerged in view of the exchange of data (text and binary) and gluing of codes :

(1) Python, as scripting language, its interfaces with C and FORTRAN;
(2) XML, a standard for representing structured data in text files;
(3) netCDF, a library and file format for the exchange and storage of binary data, and its interfaces with C, Fortran, and Python

Scientific content:

Recent discussions, related to the CECAM workshop on "Open Source Software for Microscopic Simulations", June 19-21, 2002, to the GRID concept (http://www.gridcomputing.com), as well as to the future Integrated Infrastructure Initiative proposal linked to the European Psi-k network (http://psi-k.dl.ac.uk), have made clear that one challenge for the coming years is the ability to establish standards for accessing codes, transferring data between codes, testing codes against each other, and become able to "glue" them (this being facilitated by the Free Software concept).

In the present tutorial, we would like to teach three "software solutions" to face this challenge : Python, XML and netCDF.

Python is now the de facto "scripting langage" standard in the computational physics and chemistry community. XML (eXtended Markup Language) is a framework for building mark-up languages, allowing to set-up self-describing documents, readable by humans and machines. netCDF allows binary files to be portable accross platforms. It is not our aim to cover all possible solutions to the above-mentioned challenges (e.g. PERL, Tcl, or HDF), but these three have proven suitable for atomic-scale simulations, in the framework of leading projects like CAMPOS (http://www.fysik.dtu.dk/campos), MMTK (http://dirac.cnrs-orleans.fr/MMTK), and GROMACS (http://www.gromacs.org). Other software projects like ABINIT (http://www.abinit.org)

and PWSCF (http://www.pwscf.org - in the DEMOCRITOS context), among others, have made clear their interest for these. All of these software solutions can be used without having to buy a licence.

Tentative program of the tutorial. Lectures in the morning, hands-on training in the afternoon.

1st day:

2h - Python basics
1h - Interface : Python/C or FORTRAN
1h - XML basics
Afternoon Training with Python, and interfaces with C and FORTRAN

2nd day:

2h - Python : object oriented (+ an application to GUI and Tk) 1h - Interface : Python/XML
1h - Interface : XML + C or FORTRAN
Afternoon Training with XML + interfaces

3rd day:

1h - Python : numerical
1h - netCDF basics
1h - Interface : netCDF/Python
1h - Interface : netCDF/C or FORTRAN
Afternoon Training with netCDF + interfaces

List of lecturers

K. Hinsen (Orleans, France), organizer
X. Gonze (Louvain-la-Neuve, Belgium), organizer
K. Jakobsen (Lyngby, Denmark), instructor
J. Schiotz (Lyngby, Denmark), instructor
J. Van Der Spoel (Groningen, The Netherlands), instructor
M. van Loewis (Berlin, Germany), instructor

Number of participants: around 20,

Most of the participants should be PhD students, postdoc or young permanent scientists, involved in code development. It is assumed that the attendants have a good knowledge of UNIX, and C or FORTRAN.

Our budget will allow contributing to travel and local expenses of up to 20 participants.

6 News from UK's CCP9 Programme

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

6.1 Conference Announcements

6.1.1 B.L. Györffy's Conference in Bristol

2nd Announcement

"Order and disorder in solids: alloys, magnetism and superconductivity"

A celebration of the contributions of Balazs Györffy to theories of the electronic structure of solids

Friday 11 April to Saturday 12 April 2003

Background

Balazs Györffy has made substantial contributions in several areas of solid state physics, including: metallic alloys, metallic magnetism, superconductivity and relativistic quantum effects in solid state physics. This meeting marks the occasion of his 65th birthday. Workshop talks will encompass the current state of the art in the diverse fields in which Balazs has made a major contribution.

Dates: Friday 11 April to Saturday 12 April 2003.

Location

The meeting will take place at the H H Wills Physics Laboratory, University of Bristol, Bristol, BS8 1TL, UK.

(Note that the annual CMMP Conference will take place in Belfast 6-9 April 2003, and timings will allow participants to travel from Belfast to Bristol to attend both meetings.)

Provisional programme, registration and accommodation information are now available at

http://www.phy.bris.ac.uk/research/theory/balazs-conference.htm

Deadline for registration: 17 March 2003.

7 General Workshop/Conference Announcements

7.1 Nineth WIEN Workshop

Electronic Structure Calculations of Solids with the WIEN2k Code

April 23-26, 2003

Vienna University of Technology, Austria
Chairman: Karlheinz Schwarz (TU-Vienna)
Email: kschwarz@theochem.tuwien.ac.at

First Announcement

The program package WIEN2k allows to perform electronic structure calculations using density functional theory (DFT). This workshop is aimed at anyone who wants to learn how DFT calculations can be done using the full-potential (Linearized) Augmented Plane Wave + local orbitals (FP-APW+lo) method as embodied in the WIEN2k code (or related topics). Presently this code is used worldwide by more than 500 groups from academic and industrial reserach institutions to solve many material science problems.

The workshop will include lectures, the presentation of results and exercise sessions. It consists of two parts as follows:

- Part I:
  - A short introduction into density functional theory and the (L)APW (+lo) method
  - Introduction to the use of the WIEN2k program package
  - Hands-on experience (on LINUX clusters)
- Part II:
  - New features of WIEN2k (non-linear optics, non-collinear magnetism, phonons, etc.)
  - Contributed papers, results obtained with WIEN and related topics
  - Poster session
  - Discussions and exchange of experience with users and developers

Conference site:
The conference will take place at the TU Wien (Vienna University of Technology)
A-1040 Vienna, Wiedner Hauptstr. 8

Contact:

For further details see our WWW-homepage
http://www.wien2k.at/
or send an email to kschwarz@theochem.tuwien.ac.at.

8 General Job Announcements

IFP Post-doctoral Position (Rueil-Malmaison, France)

Kinetic Monte Carlo Simulation of Catalytic Hydrodesulfurization

A post-doctoral position is available in the Department of Thermodynamics and Molecular Modeling at the IFP (Institut Francais du Petrole www.ifp.fr) under the supervision of Dr H. TOULHOAT. The proposed project involves the generation from first-principles of kinetic data, for reactions catalyzed by transition metal sulfides providing relevant models for industrial processes of paramount importance for producing clean fuels in refineries. Over the past years, our group has elaborated a significant amount of energetic data and surface configurations for the most important elementary steps of these reactions (1,10). This database should now provide the foundation for KMC simulations aiming at providing pictures of the working catalyst's surface, as well as kinetic data directly comparable with experiment. To meet this goal, it is necessary to develop system specific pieces of code on the one hand, and to define and run ab initio calculations designed to complement the existing database. The assistance of international experts in the field will be provided through existing channels of collaboration.

Eligibility: The preference will be given to non-french candidates, having defended their PhD in the past three years.

Qualification: Candidates should have a PhD and a background in the theoretical and computational methods of condensed matter physics. Experience of density functional calculations and kinetic Monte Carlo simulations is desirable.

Duration: Up to 18 months, with an initial contract of 12 months.

Application: Candidates should send, preferably by e-mail, their CV, list of publications and coordinates of a few reference persons to:

Dr H. TOULHOAT
Deputy Scientific Director
Institut Francais du Petrole
1 & 4 avenue de Bois-Preau
92852 Rueil-Malmaison Cedex
France

Tel +33 1 47 52 73 50
Fax +33 1 47 52 70 36

e-mail: herve.toulhoat@ifp.fr

References cited:

(1) P. Raybaud, G. Kresse, J. Hafner and H. Toulhoat, " Ab-initio density-functional studies of transition-metal sulfides: I. Crystal structure and cohesive properties ", J. Phys.: Condens. Matter 9, 11, 085-106 (1997).

(2) P. Raybaud, J. Hafner, G. Kresse and H. Toulhoat, " Ab-initio density-functional studies of transition-metal sulfides: II. Electronic structure ", J. Phys.: Condens. Matter 9, 11, 107-40 (1997).

(3) P. Raybaud, J. Hafner, G. Kresse and H. Toulhoat, " The adsorption of thiophene on the catalytically active edge-surface of MoS2: An ab-initio local-density-functional study ", Phys. Rev. Lett. 80, 1481-4 (1998).

(4) H. Toulhoat, P. Raybaud, S. Kasztelan, G. Kresse and J. Hafner, " Transition Metals to Sulfur Binding Energies Relationship to Catalytic Activities in HDS: back to Sabatier with First-Principles Calculations ", Catalysis Today 50 (1999) 629-636.

(5) P. Raybaud, J. Hafner, G. Kresse and H. Toulhoat, " The structural and electronic properties of the MoS2 (10-10) edge surface", Surf. Sci. 407, 237-50 (1998).

(6) P. Raybaud, J. Hafner, G. Kresse, S. Kasztelan, H. Toulhoat, " Ab initio study of the H2-H2S/MoS2 gas-solid interface: the nature of the catalytically active sites ", J. Catal. 189, 129-146 (2000).

(7) P. Raybaud, J. Hafner, G. Kresse, S. Kasztelan, H. Toulhoat, " Structure, energetics and electronic properties of the surface of a promoted MoS2 catalyst: an ab initio local-density functional study ", J. Catal. 190, 128-143 (2000).

(8) R.R. Chianelli, G. Berhault, P. Raybaud, S. Kasztelan, J. Hafner, H. Toulhoat, "Periodic trends in hydrodesulfurization: in support of the Sabatier principle", Applied Catalysis A: General 227 (2002) 83-96.

(9) H.Schweiger, P. Raybaud , G. Kresse, H.Toulhoat, "Shape and Edge Sites Modifications of MoS2 Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study", J. Catal. 207, 76-87 (2002).

(10) H.Schweiger, P. Raybaud, H.Toulhoat, " Promoter Sensitive Shapes of Co(Ni)MoS Nanocatalysts in Sulfo-Reductive Conditions", J. Catal. 212, 33-38 (2002).

EU-RTN Post-doctoral Position (Goeteborg)
Theory of Atomic and Molecular Manipulation

A post-doctoral position is available in the group of "Materials and Surface Theory". This position is funded by the EU-RTN research network "Atomic and Molecular Manipulation as a New Tool in Science and Technology" (AMMIST). The succesful candidate should work on theoretical modeling and description of problems related to manipulation of individual atoms and molecules by the scanning tunneling microscope. Main areas of interest include imaging and manipulation of nanostructures and the characterization of their chemical and physical properties. In particular, the theory of inelastic tunneling is a speciality of our group. The modeling is primarily based on density functional methods. The proposed work will be carried out in close collaboration with the theory group (C. Joachim, Toulouse) and the experimental groups of the AMMIST network (G. Dujardin, Paris; F. Besenbacher, Aarhus; G. Meyer, IBM Zurich; F. Moresco, Berlin; R. Palmer, Birmingham) and the experimental group of Wilson Ho, UCI, USA. More information about the activities and interests of the network and our group can be found at the URLs www.fy.chalmers.se/ammist and fy.chalmers.se/ap/mst.

Eligibility: You must be an national of an EU Member State or Associated State and you must be aged 35 or less at the time of your appointment to the network. For further details see `www.cordis.lu/improving/networks/faq.htm#q5`

Duration: The position is for 2-3 years and starting date is flexible.

Salary: For candidates with a PhD degree awarded no more than 2-4 years ago, we can offer a very competive taxfree fellowship.

Qualifications: Candidates should have a PhD and a background in the theoretical and computational methods of condensed matter physics. In particular, experience of density functional calculations is highly desirable.

Application: Applicants should send a CV, a list of publications, and names of a few referees to:

Prof. Mats Persson,

Material and Surface Theory, Soliden 3,
Chalmers/Göteborg Univ.,
S-412 96 Göteborg, SWEDEN

Phone office: +46-31-772-3666
FAX: +46-31-772-8426
`WWW: http://fy.chalmers.se/~tfymp`

Postdoctoral Position in Theoretical Physical Chemistry
University of Liége, BELGIUM

A post-doc position is available at the University of Liége (BELGIUM) to work jointly with Dr. F. Remacle (Theoretical Physical Chemistry) and Prof. Ph. Ghosez (Theoretical Physics of Materials).

The research project deals with the computation of the optical, electronic and transport properties of semi-conducting nanoparticles in view of their applications to nano analysis of biocompounds. Experience in ab initio and DFT computations on large clusters and in quantum semi empirical models is required.

The position is available immediately. Application (short CV + list of publications), together with names and contact information for 2 references, can be sent to

Dr. F. Remacle,
Department of Chemistry, B6c,
University of Liége,
B-4000 Liége,
Belgium

Email address : fremacle@ulg.ac.be.

Postdoctoral or Research Associate Positions
Department of Physics and Astronomy, Rutgers University

One or more postdoctoral or research associate positions may become available beginning summer or fall 2003, associated with Profs. David Langreth, Karin Rabe, and David Vanderbilt in the computational materials theory group, Department of Physics and Astronomy, Rutgers University. 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 by 1 February 2003. Email submission in the form of a postscript or pdf file is preferred.

rabe@physics.rutgers.edu

Prof. Karin Rabe
Dept. of Physics and Astronomy
Rutgers University
136 Frelinghuysen Road
Piscataway, NJ 08854-8019
USA
fax: 1-732-445-4343

Postdoctoral/Research Associate Positions In Electronic Structure Theory

National Renewable Energy Laboratory (NREL)

`http://www.sst.nrel.gov`

NREL's Solid State Theory Group is looking to fill two postdoctoral/research associate positions in the area of Electronic Structure Theory. The positions are for 2-3 years. The salary range is USD 45,000 - USD 60,000/year, depending on qualifications and rank (postdoc vs. research associate). Applicants are expected to have a strong background in solid-state theory. The positions are with Alex Zunger, Solid State Theory Group Leader, and involve working in either (a) Quantum Dot Physics, or; (b) Physics of Semiconductor and Metal Alloys. The start date is during the fall of 2003, but the decision on the positions will be made around 3/2003. Applications for both positions are considered now. More details about ongoing work are included in `http://www.sst.nrel.gov`.

The Solid State Theory Group currently consists of ten Ph.D.'s in condensed matter theory (see an online list of current and past personnel in the group) and interacts with a broad range of experimentalists. Furthermore, the group has outstanding computational facilities: a dedicated local computing system consisting of a 16 node SGI Origin 2000, a 20 processor Linux cluster, 4 Sun Ultra 80 workstations and remote access to IBM-SP supercomputers at NERSC, Berkeley. The group has an excellent basic-research atmosphere, and is located in the beautiful Rocky Mountains. Consult our web page for additional information on the group, its history, research subjects, publications, and facilities.

Interested candidates should send immediately curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two-three references addressed to:

Alex Zunger
Solid State Theory Group
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401

Clarification or further details can be obtained via email to azunger@nrel.gov.

NREL is an equal opportunity employer and proud of its commitment to diversity. Women and minorities are encouraged to apply.

Postdoctoral Research and PhD Positions
The Computational Modelling Group, NMRC, Ireland

The Computational Modelling Group, NMRC, Ireland has several postdoctoral research and PhD positions open.

We seek candidates with a background in theoretical physics/ chemistry, and an interest in scientific computing, electronic strucure theory, atomic scale simulation, and/or technology computer aided design. Successful candidates will pursue research projects on the following topics:

* electronic properties of fullerenes and semiconductor nanostructures
oxide film growth and structure
electronic transport/electronic structure theory
multi-scale simulation (atomic scale coupled to finite element models)

NMRC is Ireland's largest research centre with a staff of over 220 and has extensive fabrication, characterisation and computational facilities. The NMRC hosts over 40 postgraduate students pursuing postgraduate education in science and engineering on a variety of topics. The NMRC is active in research in Information & Communication Technologies, Nanotechnologies and Biotechnologies. (http://www.nmrc.ie) There is a large theory and modelling effort ongoing in Cork offering many opprortunities for collaboration and a stimulating research environment. These acrivities include the Computational Modelling Group, the Photonics Theory Group (led by E. P. O'Reilly) and University College Cork's Condensed Matter Theory Group (led by S. Fahy).

NMRC is located in Cork, the second city of the Irish republic (http://www.cork-guide.ie/corkcity.htm) and is a city of with a population of 170,000 (of which about 30,000 are students), with a lively city centre. The city offers a variety of entertainment options with traditional pubs, cafes and restaurants. Cork is situated amidst some of Ireland's most scenic regions.

Interested applicants should contact

Dr. Jim Greer, Group Director - Computational Modelling, NMRC, University College, Lee Maltings, Prospect Row, Cork, Ireland

E-mail: Jim.Greer@nmrc.ie
Telephone: +353 21 4904345
FAX: +353 21 4270271

WWW: http://www.nmrc.ie/research/computational-modelling-group/index.html

POST DOCTORAL OPENING FOR COMPUTATIONAL QUANTUM CHEMIST

Chemistry Department, Case Western Reserve University, Cleveland OH 44106 USA

The above position is available in the lab of Professor A. B. Anderson. The research centers on the determination of electrode potential-dependent reaction pathways and activation energies for electron transfer by means of constrained variational theory. Applications will be made to the electro-catalytic reduction of oxygen by copper enzymes. The appointment is for one year and may extend, contingent on funding. Please apply to aba@po.cwru.edu with cv and arrange for three letters of recommendation to be sent. It is the intention to fill the position as soon as possible.

Case Western Reserve University is an equal opportunity, affirmative action employer and encourages applications from women and minorities.

Postdoctoral Position in Computational Condensed Matter Physics

College of William and Mary, Williamsburg, VA 23187, USA

The College of William and Mary invites applicants for a post-doctoral position in the computational condensed matter physics group of Prof.'s Henry Krakauer and Shiwei Zhang. The primary focus of the work will be on the application and development of quantum Monte Carlo methods to study ferroelectric and related materials. Familiarity with ab-initio density-functional, quantum Monte Carlo, or quantum chemistry methods is highly desirable. The group has broad interests in the general area of computer calculations of quantum many-body systems. Additional information can be found at

`http://physics.wm.edu/~krakauer`

`http://physics.wm.edu/~shiwei`

`http://www.cpd.wm.edu/.`

Candidates should e-mail a CV (as a pdf attachment) with names and contact information for two or three references to

krakauer@physics.wm.edu

as soon as possible. Review of candidates will begin immediately and continue until the position is filled.

The College of William and Mary is an equal opportunity, affirmative action employer.

Advertisement for a Staff Position in NRL (Code 6390)

The Center for Computational Materials Science at the Naval Research Laboratory invites applications for a staff Level III position in computational materials or solid state science. The successful applicant will be selected from one or more of the following areas: electronic structure methods and applications, quantum Monte Carlo, dynamical mean field theory, empirical or model potentials , molecular dynamics simulations,and photonic semiconductor theories. A Ph.D. in physics,or materials science is desired.

Salary range: USD 46,040 - USD 86,262.

Deadline for applications is January 31, 2003.

Interested candidates should view Vacancy Announcement DM-NRL-02-0928-NR at

http://www.donhr.navy.mil or http://www.usajobs.opm.gov

for instructions on how to apply for the position. The Department of Navy is an Equal Opportunity Employer.

The above announcement will appear in the January issue of Physics Today. The Web site will also be open Jan 1, 2003. If you have a suitable candidate advice him/her to respond to the above address and in addition to send a copy of the application to me. Thank you for your assistance in this matter.

Dr. D.A. Papaconstantopoulos
Head, Code 6390
Center for Computational Materials Science
Naval Research Laboratory
Washington DC 20375, USA

tel 202-767-6886
fax 202-404-7546
e-mail:papacon@dave.nrl.navy.mil

PhD: Computational Chemistry

Department of Chemistry, Cambridge, UK

"Electronic States of Organic Molecules in the Condensed Phase"

An EPSRC-sponsored PhD studentship is available to work on the application of a combination of density functional and molecular dynamics methods ("Car-Parrinello") in a study of the electronic states of organic molecules in the condensed phase (liquids or solids). The objective is to understand how the coupling between the electronic states of molecules affects observable electronic properties such as ionization (redox) potentials and electronic absorption spectra, and, conversely, how to interpret the corresponding experimental data in terms of single molecule states.

Applicants should have a good honours degree (at least II.1 or equivalent) in chemistry or physics, with an interest in computational chemistry. Full funding (fees and maintenance) is available to UK citizens, and fees-only awards are available to other EU citizens.

Applications should include a CV and the names and addresses of two referees, and should be sent to Dr Michiel Sprik, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW (email: ms284@cam.ac.uk).

Post-doctoral Research Associate

Department of Chemistry, University of Cambridge

Theoretical Modelling of Nanocrystalline Materials

Applicants are invited for a postdoctoral position funded by the Leverhulme Trust to develop new methods for simulating ionic crystals encapsulated in single-walled nanotubes. This project is closely linked to an experimental programme investigating the novel structures produced by encapsulation.

The successful applicant will have a PhD in physics, chemistry or materials science and have experience in either classical simulation methods or electronic structure calculations. Some ability and experience in computer programming is essential, whilst a knowledge of Fortran is highly desirable.

The project is a collaboration between Drs Pyper (Cambridge), Harding (UCL), Kirkland (Oxford) and Professor Johnson (Cambridge). The successful applicant will be based in Cambridge, but will need to make some extended visits to UCL.

The post is available from 1st April 2003 and will be for up to three years. Salary will be in the range 18265 to 27339 GBP pa according to experience.

Informal enquiries may be made to Dr Pyper (ncp1@cus.cam.ac.uk) or Dr Harding (j.harding@ucl.ac.uk). Applications including a CV and the names of two referees should be sent to Dr Nicholas Pyper, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW (tel: 01223 336483; email: ncp1@cus.cam.ac.uk).

Closing date: February 10th 2003

The University of Cambridge is committed to equality of opportunity.

Application are invited for a

Postdoctoral Position at LCM3B, Nancy - France

"ANALYSIS OF PROTEIN - LIGAND INTERACTIONS IN THE CRYSTAL STRUCTURE AT 0.65 Å RESOLUTION"

The fellowship is funded by CNRS-DFG. German citizens have priority but applicants from other European countries can also apply. A background in Protein Crystallography, Charge Density or Molecular Modelling/Quantum Chemistry or Software Development is required. The fellowship can be started anytime in 2003 and the duration is 1 year.

X-ray crystallography at ultra high resolution reveals the deformation of the atomic electron cloud due to covalent bonds and interactions between atoms. This aspherical electron density and the resulting properties (potential, interaction energy) can be modelled and accurately estimated using the software MOPRO (MOlecular PROperties) written in our laboratory . Crystallographic data at an exceptionally ultra high resolution (0.65 Å) have been collected for a complex of aldose reductase with NADP+ and an inhibitor. Diffraction data sets with several other inhibitors are also available at 0.8 to 0.9 Å resolution. This enzyme is a pharmacological target in the treatment of diabetis complications.

The postdoctoral researcher will join the High Resolution Protein Crystallography team and the project involves:

- Ultra High Resolution Structure refinement of the Aldose Reductase Complexes

- the Development of new Methods for Molecular Recognition Analysis and participation to MOPRO Software programming.

Contact :

Christian Jelsch, jelsch@lcm3b.uhp-nancy.fr
Claude Lecomte, lecomte@lcm3b.uhp-nancy.fr

http://www.lcm3b.u-nancy.fr

Laboratoire de Cristallographie et Modélisation des Matériaux
Minéraux et Biologiques (LCM3B)
CNRS Faculté de Sciences
Bd des Aiguillettes BP 239
54 506 Vandoeuvre-les-Nancy
France

9 Abstracts

Cation site occupancy in spinel ferrites studied by X-ray magnetic circular dichroism: developing a method for mineralogists

R.A.D. Pattrick[1], G. van der Laan[2], C.M.B. Henderson[1], P. Kuiper[2], E. Dudzik[2], D.J. Vaughan[1]

[1] *Department of Earth Sciences, University of Manchester, Manchester SK17 9BB, UK*

[2] *Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK*

Abstract

X-ray magnetic circular dichroism (XMCD) is an element-, site- and symmetry-selective spectroscopic technique that has the potential to provide quantitative information on site occupancies in ferri- and ferro-magnetic minerals. XMCD spectra derived from the Fe $L_{2,3}$ absorption edge of a series of synthetic spinel ferrites and natural magnetite were collected using synchrotron radiation and a 0.6 Tesla 'flipper' magnet. These spectra were used to assess their potential value to mineralogical investigations. By comparison with theoretical spectra, the site occupancies of the cations have been calculated and compared to previous studies using other techniques. The spectra of the Co, Ni, Zn and Mg ferrite spinels show considerable variation, reflecting differences in site occupancies. Although the cation ratios derived from the XMCD spectra are broadly similar to previous work, there are significant differences especially in the amount of octahedral Fe^{2+} present. Incomplete inversion is recognised in all the spinels analysed and the affinity of Co, Ni and Mg for the octahedral site and Zn for the tetrahedral site is confirmed; the preference of Co over Ni for tetrahedral sites is also revealed. XMCD spectra proved relatively straightforward to analyse but further refinement of the quantitative calculations is needed and detailed comparison with the information derived from other methods, especially Mossbauer spectroscopy.

(EUROPEAN JOURNAL OF MINERALOGY 14 (6): 1095-1102 NOV-DEC 2002)
Contact person: g.vanderlaan@dl.ac.uk

Improving the convergence of defect calculations in supercells - an *ab initio* study of the neutral silicon vacancy

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Heslington, York, YO10 5DD, U.K.
M C Payne
Cavendish Laboratory, University of Cambridge,
Madingley Road, Cambridge, CB3 0HE, U.K.

Abstract

We present a systematic methodology for the accurate calculation of defect structures in supercells which we illustrate with a study of the neutral vacancy in silicon. This is a prototypical defect which has been studied extensively using *ab initio* methods, yet remarkably there is still no consensus about the energy or structure of this defect, or even whether the nearest neighbour atoms relax inwards or outwards. In this paper we show that the differences between previous calculations can be attributed to supercell convergence errors, and we demonstrate how to systematically reduce each such source of error. The various sources of scatter in previous theoretical studies are discussed and a new effect, that of supercell symmetry, is identified. It is shown that a consistent treatment of this effect is crucial to understanding the systematic effects of increasing the supercell size. This work therefore also presents the best converged *ab initio* study of the neutral silicon vacancy to date.

(Accepted, Phys. Rev. B)
Contact person: mijp1@york.ac.uk

Short hydrogen-hydrogen separation in RNiInH$_{1.333}$

P. Vajeeston[1], P. Ravindran[1], R. Vidya[1], A. Kjekshus[1], H. Fjellvåg[1,2], and V.A. Yartys[2]

[1] *Department of Chemistry, University of Oslo,*
Box 1033, Blindern, N-0315, Oslo, Norway

[2] *Institute for Energy Technology, N-2027 Kjeller, Norway*

Abstract

First principle studies on the total energy, electronic structure and bonding nature of RNiIn (R = La, Ce and Nd), and their saturated hydrides ($R_3Ni_3In_3H_4$ = RNiInH$_{1.333}$) are performed using a full-potential linear muffin-tin orbital approach. This series of phases crystallizes in a ZrNiAl-type structural frame-work. When hydrogen is introduced in the RNiIn matrix, anisotropic lattice expansion is observed along [001] and lattice contraction along [100]. In order to establish the equilibrium structural parameters for these compounds we have performed force minimization as well as volume and c/a optimization. The optimized atomic positions, cell volume and c/a ratio are in very good agreement with recent experimental findings. From the electronic structure and charge density, charge difference, electron localization function analyses the microscopic origin of the anisotropic change in lattice parameters on hydrogenation of RNiIn has been identified. The hydrides concerned, with their theoretically calculated interatomic H-H distances of ~ 1.57 Å, violate the "2 Å rule" for H-H separation in metal hydrides. The shortest inter-nuclear Ni-H separation is almost equal to the sum of the covalent radii. H is bonded to Ni in an H-Ni-H dumb-bell shaped linear array, with a character of NiH_2 subunits. Density of states, valence charge density, charge transfer plot and electron localization function analyses clearly indicate significant ionic bonding between Ni and H and weak metallic bonding between H-H. The paired, localized, and bosonic nature of the electron distribution at the H site is polarized towards La and In which reduces the repulsive interaction between negatively charged H atoms. This could explain the unusually short H−H separation in these materials. The calculations show that all these materials have metallic character.

(Accepted for publication Phys. Rev. B)

Contact person: ravindran.ponniah@kjemi.uio.no

The ab-initio ground state properties and magnetic structure of plutonium

A.L. Kutepov and S.G. Kutepova
Institute of Technical Physics, Snezhinsk, Chelyabinsk Region, Russia

Abstract

With the RSPFLAPW (fully relativistic spin-polarized full potential linearized augmented plane wave) method we calculate the energy differences, the ground state properties and magnetic moments of alpha- and delta-plutonium with different alignment of the atomic magnetic moments. We have found that alpha-plutonium with some magnetic structure has the lowest total energy at experimental equilibrium volume. This magnetic structure has ferrimagnetic ordering of the atomic magnetic moments with the immensely small value of the total magnetic moment or the antiferromagnetic ordering. As the authors of the series of earlier works we found the antiferromagnetic structure of delta-plutonium has the lowest total energy among others magnetic and nonmagnetic phases of delta-plutonium. But we have obtained the quite right ground state properties for this phase without taking into account of the orbital polarization. An important conclusion from the given work is the taking into account of the spin polarization severely improves the calculated ground state properties of both alpha- and delta-plutonium.

(Submitted to J.Physics of Condensed Matter)
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Calculation of bulk moduli of semiconductor compounds

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Abstract

The bulk modulus has been calculated by using the energy gapalong Γ-X and the transition pressure for diamond and zinc-blende semiconductors. The obtained order of magnitude is in reasonable agreement with experimental and other calculations.

(Physica B 322 (2002) 179-182)
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The effect of pressure on the ionicity of In-V compounds

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Abstract

A study of the ionicity factor under hydrostatic pressure for InSb, InAs and InP is presented. This factor has been calculated by means of an empirical model. The structural phase transition is related to the behavior of the bonding character. The results are compared with other theoretical calculations and experimental data and are in reasonable agreement.

(Physica B 324 (2002) 173-178)
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Effects of Crystal Structure and On-Site Coulomb Interactions on the Electronic and Magnetic Structure of Pyrochlores $A_2Mo_2O_7$ (A= Y, Gd, and Nd)

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Abstract

Being motivated by recent experimental studies, we investigate magnetic structures of the Mo pyrochlores $A_2Mo_2O_7$ (A= Y, Nd, and Gd) and their impact on the electronic properties. The latter are closely related with the behavior of twelve Mo(t_{2g}) bands, located near the Fermi level and well separated from the rest of the spectrum. We use a mean-field Hartree-Fock approach, which combines fine details of the electronic structure for these bands, extracted from the conventional calculations in the local-density approximation, the spin-orbit interaction, and the on-site Coulomb interactions amongst the Mo($4d$) electrons, treated in the most general rotationally invariant form. The Coulomb repulsion U plays a very important role in the problem, and the semi-empirical value $U\sim$1.5-2.5 eV accounts simultaneously for the metal-insulator (M-I) transition, the ferromagnetic (FM) - spin-glass (SG) transition, and for the observed enhancement of the anomalous Hall effect (AHE). The M-I transition is mainly controlled by U. The magnetic structure at the metallic side is nearly collinear FM, due to the double exchange mechanism. The transition into the insulating state is accompanied by the large canting of spin and orbital magnetic moments. The sign of exchange interactions in the insulating state is controlled by the Mo-Mo distances. Smaller distances favor the antiferromagnetic coupling, which preludes the SG behavior in the frustrated pyrochlore lattice. Large AHE is expected in the nearly collinear FM state, near the point of M-I transition, and is related with the unquenched orbital magnetization at the Mo sites. We also predict large magneto-optical effect in the same FM compounds.

(Submitted to Phys. Rev. B)
Manuscripts available from: igor.solovyev@aist.go.jp or cond-mat/0211615.

Is Charge Ordering Responsible for the "Charge-Ordered" Phase of Manganites?

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Abstract

It is argued that both transitions observed in the 50%-doped manganites, at the Néel temperature ($T_{\rm N}$) and the so-called charge ordering temperature ($T_{\rm CO}$), are magnetic. $T_{\rm N}$ corresponds to the order-disorder transition, which takes place between ferromagnetic zigzag chains. The coherent motion of spins within each chain is destroyed only around $T_{\rm CO}$, which corresponds to the transition to the totally disordered paramagnetic state. The behavior is related with the anisotropy of the electronic structure, which accompanies this highly anisotropic magnetic state and naturally explains the appearance of charge-orbital superstructures above $T_{\rm N}$. The type of the phase transition at $T_{\rm N}$ depends on the Jahn-Teller distortion.

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Manuscripts available from: igor.solovyev@aist.go.jp or cond-mat/0212608

Aspects of layer-by-layer composition analysis using MEIS

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Abstract

The shadowing/blocking characteristics of medium energy ion scattering allow a precise deduction of the layer-by-layer composition of alloy crystal surfaces. The technique relies on an accurate alignment of the ion beam with known crystallographic directions to restrict the incoming beam to illuminate just the topmost one, two or three or more layers. Further layer specificity is bestowed by utilising outgoing geometries that block ions from all but the top one, two, etc., layers respectively. The size of shadow cones associated with medium energy hydrogen and helium ions is ideal for this application. A plot of the averaged experimental yields against simulated yields for several di.erent systems implies an inconsistency in the technique. Possible explanations for this are discussed and a clarifying experiment is suggested.

(Submitted to Current Applied Physics)

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Ga adsorption on (0001) GaN surfaces

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Abstract

We study the adsorption behavior of Ga on (0001) GaN surfaces combining experimental specular reflection high-energy electron diffraction with theoretical investigations based on an *ab initio* based growth model. Based on the experimental results we find that, for substrate temperatures and Ga fluxes typically used in molecular-beam epitaxy of GaN, dynamically-stable *finite* Ga surface coverages can be obtained. The measurement of a Ga/GaN adsorption isotherm allows to quantify these Ga surface coverages as a function of the impinging Ga flux. In particular, we show that a large range of Ga fluxes exists, where 2.5 ± 0.2 monolayers (in terms of the GaN surface site density) of Ga are adsorbed on the GaN surface. We further demonstrate that the structure of this adsorbed Ga film is in good agreement with the laterally-contracted Ga bilayer model found to be most stable for strongly Ga-rich surfaces [J. E. Northrup *et al.*, Phys. Rev. B **61**, 9932 (2000)]. For lower Ga fluxes, a discontinuous transition to monolayer coverage is found, followed by a continuous decrease towards zero coverage; for higher Ga fluxes, Ga droplet formation is found, similar to what has been observed during Ga-rich GaN growth. The boundary fluxes limiting the region of 2.5 ML steady-state Ga adsorption have been measured as a function of the GaN substrate temperature giving rise to a Ga/GaN adsorption phase diagram. The temperature dependence is discussed in the framework of an *ab initio* based growth model for adsorption taking into account the nucleation of Ga clusters. This model consistently explains recent contradictory results on the critical Ga flux for the onset of Ga droplet formation during Ga-rich GaN growth [B. Heying *et al.*, J. Appl. Phys. **88**, 1855 (2000); C. Adelmann *et al.*, J. Appl. Phys. **91**, 9638 (2002).].

(submitted to: Phys. Rev. B)
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Morphology and surface reconstructions of m-plane GaN

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Abstract

M-plane GaN($10\bar{1}0$) is grown by plasma assisted molecular beam epitaxy on ZnO($10\bar{1}0$) substrates. A low-temperature GaN buffer layer is found to be necessary to obtain good structural quality of the films. Well oriented ($10\bar{1}0$) GaN films are obtained, with a slate like surface morphology. On the GaN($10\bar{1}0$) surfaces, reconstructions with symmetry of c(2×2) and approximate "4×5" and are found under N- and Ga-rich conditions, respectively. We propose a model for Ga-rich conditions with the "4×5" structure consisting of ≥ 2 monolayers of Ga terminating the GaN surface.

MRS symp. proc. (in print)
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Morphology and surface reconstructions of GaN$(1\bar{1}00)$ surfaces

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Abstract

GaN is grown by plasma assisted molecular beam epitaxy on ZnO$(1\bar{1}00)$ substrates. Well-oriented $(1\bar{1}00)$ GaN surfaces are obtained, and $(1\bar{1}01)$ oriented facets are also observed. On the GaN$(1\bar{1}00)$ surfaces under Ga-rich conditions a surface reconstruction with approximate symmetry of "4×5" is found. A model is proposed in which this reconstruction consists of ≥ 2 monolayers of Ga terminating the GaN surface.

(submitted to: Appl. Phys. Lett.)
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Why is a noble metal catalytically active? The role of the O-Ag interaction in the function of silver as an oxidation catalyst

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Abstract

Extensive density-functional theory calculations, and taking into account temperature and pressure, affords a comprehensive picture of the behavior and interaction of oxygen and Ag(111), and provides valuable insight into the function of silver as an oxidation catalyst. The obtained phase-diagram reveals the most stable species present in a given environment and thus identifies (and excludes) possibly active oxygen species. In particular, for the conditions of ethylene epoxidation, a thin oxide-like structure is most stable, suggesting that such atomic O species are actuating the catalysis, in contrast to hitherto proposed molecular-like species.

(submitted to: Phys. Rev. Lett.)
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First-principles, atomistic thermodynamics for oxidation catalysis: Surface phase diagrams and catalytically interesting regions

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Abstract

Present knowledge of the function of materials is largely based on studies (experimental and theoretical) that are performed at low temperatures and ultra-low pressures. However, the majority of everyday applications, like e.g. catalysis, operate at atmospheric pressures and temperatures at or higher than 300 K. Here we employ *ab initio*, atomistic thermodynamics to construct a phase diagram of surface structures in the (T, p)-space from ultra-high vacuum to technically-relevant pressures and temperatures. We emphasize the value of such phase diagrams as well as the importance of the reaction *kinetics* that may be crucial e.g. close to phase boundaries.

Phys. Rev. Lett. (in press)
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Surface Coordination Chemistry: Dihydrogen versus Hydride Complexes on $RuO_2(110)$

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Abstract

Similarities between bond formation in transition metal complexes and chemisorption on solid surfaces form the basis for relations between homogeneous and heterogeneous catalysis. Coupling of hydrogen is generally associated with dissociation of the ligand. We find that hydrogen interacts in a complex manner with the two under-coordinated sites Ru^{cus} and O^{bridge} on the $RuO_2$2(110) surface. Upon exposure at 85 K, H_2 instead of dissociating at Ru^{cus} weakly adsorbs as dihydrogen on top of Ru^{cus} and dissociatively interacts with O^{bridge} in forming a metastable dihydride (waterlike) complex which upon further heating transforms into the stable monohydride. The combination of low-temperature ultrahigh vacuum experiments in conjunction with DFT calculations provides detailed insights into the coordination chemistry of a solid surface which, on the other hand, exhibits remarkable correlations to complex chemistry with single transition metal atoms.

(submitted to: Angew. Chemie Int. Ed.)
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Curie temperatures of III-V diluted magnetic semiconductors calculated from first-principles

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Abstract

Curie temperatures of the diluted magnetic semiconductors (Ga, Mn)As, (Ga, Mn)N, (Ga, Cr)As and (Ga, Cr)N are evaluated from first-principles. The electronic structure is calculated in the local spin density approximation by using the Korringa-Kohn-Rostoker method combined with the coherent potential approximation to describe the substitutional and spin disorder. From the total energy differences between the ferromagnetic state and the spin-glass state, realistic estimations of Curie temperatures are achieved by using a mapping on the Heisenberg model in the mean field approximation. Effects of additional carrier doping treatments are also investigated. Very large Curie temperatures are obtained, lying above room temperature for (Ga, Mn)N, (Ga, Cr)As and (Ga, Cr)N. Upon hole doping the Curie temperature of (Ga, Mn)N further increases, while (Ga, Mn)As shows a plateau behavior.

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Exchange interactions in diluted magnetic semiconductors

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Abstract

Based on *ab initio* calculations for Mn-doped GaN, GaP, GaAs and GaSb, we discuss the origin of ferromagnetism in diluted magnetic semiconductors. The calculations use the Korringa-Kohn-Rostoker method in connection with the coherent potential approximation to describe the substitutional and moment disorder. By mapping the total energy results on a Heisenberg model, the Curie temperature $T_{\rm C}$ is estimated in the mean field approximation. If impurity bands are formed in the gap, as it is the case for (Ga, Mn)N, double exchange dominates leading to a characteristic $\sqrt{c}$-dependence of $T_{\rm C}$ as a function of the Mn concentration c. On the other hand, if the d-states are localized, as in (Ga, Mn)Sb, Zener's p-d exchange prevails resulting in a linear c-dependence of $T_{\rm C}$. (Ga, Mn)As is an intermediate case, showing a $\sqrt{c}$-like behavior in the local density approximation (LDA), but a nearly linear c-dependence, if the LDA+U method, with $U = 4$ eV, is used.

(Submitted to Phys. Rev. Lett.)
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Zinc-blende compounds of transition elements with N, P, As, Sb, S, Se, and Te as half-metallic systems

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Abstract

We report systematic first-principles calculations for ordered zinc-blende compounds of the transition metal elements V, Cr, Mn with the *sp* elements N, P, As, Sb, S, Se, Te, motivated by recent fabrication of zinc-blende CrAs, CrSb, and MnAs. They show ferromagnetic half-metallic behavior for a wide range of lattice constants. We discuss the origin and trends of half-metallicity, present the calculated equilibrium lattice constants, and examine the half-metallic behavior of their transition element terminated (001) surfaces.

(To be published in Phys. Rev. B)
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Thermodynamics of charged surfaces from density functional theory: Application to missing-row reconstruction of Pt(110) and Au(110)

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Abstract

The stability of missing-row reconstructions of (110) surfaces with respect to surface charging has been investigated using *ab initio* theory, taking Pt and Au as representative systems. We address the question of whether a positive (negative) surface charge can lift (induce) the reconstruction, or at least provide any monotonic trend in this respect. This turns out not to be the case, either in constant charge, or in constant potential mode. Instead the following consistent picture arises: at small surface charges, the effect of the charge follows the difference of the work functions, i.e. positive charge favours the surface having the smaller work function, and *vice versa*. Larger charges, either positive or negative, tend to stabilise the reconstructed surface, or more generally, the $1 \times r$ reconstruction with larger r. The approach that we use in the present study allows us to relate conveniently quantities computable from first-principles calculations to those commonly used in the thermodynamics of charged electrodes.

(Submitted to Phys. Rev. B)

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Adsorption-induced lifting of the Pt(110) (1×2) reconstruction: an *ab-initio* study

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Abstract

CO adsorption on Pt(110) (1×2) and (1×1) has been studied using *ab initio* density functional theory. Energetically, we find that the adsorption lifts the reconstruction at a coverage in the vicinity of 0.5 ML. The calculations show that the primary driving force is the increased on-site binding energy on the (1×1) surface. At 0.5 ML, we find a remarkable CO-CO attraction on the (1×1) surface, leading to the formation of chains aligned along [001]. This effect contributes to the relative destabilisation of the (1×2) surface, and appears to have a through-substrate origin.

(Submitted to Phys. Rev. Lett.)
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An embedded Green-function approach to the ballistic electron transport through an interface

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Abstract

We present an efficient method for calculating the conductance of ballistic electrons through an interface from first-principles using the embedding approach of Inglesfield. In our method the Landauer-Büttiker formula for ballistic transport is expressed in terms of two quantities that are available in the embedded Green-function formalism without additional calculations. One is the embedding potential of bulk crystals on both sides of the interface and the other is the Green function in the interface region. As a proof of principle we calculate on the basis of the density functional theory the spin-resolved electron transmission through a model system of ferromagnetic Co monolayers sandwiched between bulk Cu crystals. The relationship between our formulation and the Green-function formulation of Baranger and Stone is discussed.

Phys. Rev. B **66**, 075113 (2002)
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Ab initio theory of exchange interactions and the Curie temperature of Gd metal

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Abstract

An *ab initio* approach to magnetic properties of bulk hexagonal Gd is developed that is based on the local spin-density approximation with the $4f$ electrons treated as localized core electrons. The effective one-electron problem is solved using the tight-binding linear muffin-tin orbital method in the atomic-sphere approximation with the valence basis consisting of s-, p-, and d-type orbitals. The approach leads to a correct description of ground-state properties like the stability of ferromagnetic structure, the magnetic moment and the equilibrium lattice constant. Application of a real-space Green-function formalism yields the exchange pair interactions that are inevitable for quantitative studies of magnetic excitations. The distance dependence and anisotropy of the exchange pair interactions are presented and the Curie temperature in the mean-field approximation is evaluated. The obtained value of 334 K is in a much better agreement with the experimental value of 293 K than previous theoretical results.

(Submitted to J. Phys.: Condensed Matter)
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A fist-principles study of electronic structure and exchange interactions in bcc europium

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Abstract

Magnetic properties of the europium metal in a bcc structure are studied from first principles using a two-step approach. First, the electronic structure of the ferromagnetic state is calculated in the local spin-density approximation (LSDA) to the density-functional theory whereby the highly localized $4f$ orbitals are treated as part of the atomic core. This description leads to an equilibrium lattice constant that compares well with experiment, in contrast to the standard LSDA which yields a significantly smaller atomic volume. In the second step, parameters of an effective Heisenberg Hamiltonian are derived from the selfconsistent electronic structure and they are used to determine the magnetic ground state and to estimate the magnetic transition temperature. The calculated pairwise exchange interactions tend to couple the local magnetic moments of the nearest neighbors ferromagnetically. However, the interaction parameters exhibit a slow oscillatory decay as a function of the interatomic distance which makes them fully compatible with an observed spin-spiral ground state. The resulting wave vector of the spiral as well as the Néel temperature are in fair agreement with measured values.

(Submitted to Phys. Rev. B)
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Strain-induced surface structures on Ge(111):Sb(1 ML)

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Abstract

STM images of surface structures of an Sb-covered Ge film growing on Si(111):Sb are presented, showing the $(\sqrt{3} \times \sqrt{3})$ structure on Si(111):Sb, finite size hexagons with facets of (1×1) structure for 3 monolayers Ge, and the (2×1) structure for the thick relaxed Ge film. Using an *ab initio* total energy and force method, we have investigated the stability of the different structures of Ge(111):Sb(1 ML) as a function of the lateral lattice constant. We find that the (2×1) chain-reconstruction of Ge(111):Sb experimentally found to be stable at the equilibrium lattice constant of Ge has a range of stability between about 5.5% compression and 1% expansion. For larger dilatations the (1×1)-structure becomes stable, for larger compressions the T_4 $(\sqrt{3} \times \sqrt{3})$ structure. The observed (1×1)-structure on top of the hexagons can be explained by an over-relaxation of the surface due to the additional dilatational strain exerted by Sb atoms at the rim of the finite islands.

(Submitted to Europhys. Lett.)
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Element Specific Surface Reconstructions of Islands During Surfactant-Mediated Growth on Si(111)

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Abstract

The early stages of surfactant (As, Sb) mediated homoepitaxial growth on Si(111) are examined by scanning tunneling microscopy and extensive *ab initio* calculations of Si_n-clusters ($n \leq 12$). The results reveal the different microscopic behavior of the two surfactants: On As-covered Si(111), one exclusively finds two-dimensional islands with double-layer height which show the (1×1) terrace structure. On Sb-covered Si(111) the islands show two different reconstructions: at the rim of the islands a (1×1)-structure appears, while in the center the $(\sqrt{3}\times\sqrt{3})$ terrace structure is observed. ¿From the calculations we conclude that double layer growth on Si(111):Sb (1×1) is energetically unfavorable, and on Si(111):Sb $(\sqrt{3}\times\sqrt{3})$ it is hindered by a large kinetic barrier of 1 eV for the nucleation of Sb-trimers in the second layer.

(Phys. Rev. Lett. **89**, 236101 (2002))
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Exploring dynamical magnetism with time-dependent density-functional theory: from spin fluctuations to Gilbert damping

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Abstract

We use time-dependent spin-density-functional theory to study dynamical magnetic phenomena. First, we recall that the local-spin-density approximation (LSDA) fails to account correctly for magnetic fluctuations in the paramagnetic state of iron and other itinerant ferromagnets. Next, we construct a gradient-dependent density functional that does not suffer from this problem of the LSDA. This functional is then used to derive, for the first time, the phenomenological Gilbert equation of micromagnetics directly from time-dependent density-functional theory. Limitations and extensions of Gilbert damping are discussed on this basis, and some comparisons with phenomenological theories and experiments are made.

(Europhys. Lett. **61**, p. 354 (2003))

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Density-functional study of the Mott gap in the Hubbard model

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Abstract

We study the Mott insulating phase of the one-dimensional Hubbard model using a local-density approximation (LDA) that is based on the Bethe Ansatz (BA). Unlike conventional functionals the BA-LDA has an explicit derivative discontinuity. We demonstrate that as a consequence of this discontinuity the BA-LDA yields the correct Mott gap, independently of the strength of the correlations. A convenient analytical formula for the Mott gap in the thermodynamic limit is also derived. We find that in one-dimensional quantum systems the contribution of the discontinuity to the full gap is more important than that of the band-structure gap, and discuss some consequences this finding has for electronic-structure calculations.

(Europhys. Lett. **60**, p. 601 (2002))

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Comment on "Anomalous proximity effect in underdoped $YBa_2Cu_3O_{6+x}$ Josephson junctions

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Abstract

In recent photodoping experiments Decca et al. [PRL 85, 3708 (2000)] have observed an unusually long-ranged proximity effect between the superconducting and insulating phases of YBCO. Here we critically examine the claim in that reference that such long range is anomalous. We show that, once the novel nature of the experiments has been properly accounted for, the conventional theory of the proximity effect predicts comparably long ranges.

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Density-functional theory for the Hubbard model: numerical results for the Luttinger liquid and the Mott insulator

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Abstract

We construct and apply an exchange-correlation functional for the one-dimensional Hubbard model. This functional has built into it the Luttinger-liquid and Mott-insulator correlations, present in the Hubbard model, in the same way in which the usual *ab initio* local-density approximation (LDA) has built into it the Fermi-liquid correlations present in the electron gas. An accurate expression for the exchange-correlation energy of the homogeneous Hubbard model, based on the Bethe Ansatz (BA), is given and the resulting LDA functional is applied to a variety of inhomogeneous Hubbard models. These include finite-size Hubbard chains and rings, various types of impurities in the Hubbard model, spin-density waves, and Mott insulators. For small systems, for which numerically exact diagonalization is feasible, we compare the results obtained from our BA-LDA with the exact ones, finding very satisfactory agreement. In the opposite limit, large and complex systems, the BA-LDA allows to investigate systems and parameter regimes that are inaccessible by traditional methods.

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Density-functionals not based on the electron gas: Local-density approximation for a Luttinger liquid

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Abstract

By shifting the reference system for the local-density approximation (LDA) from the electron gas to other model systems one obtains a new class of density functionals, which by design account for the correlations present in the chosen reference system. This strategy is illustrated by constructing an explicit LDA for the one-dimensional Hubbard model. While the traditional *ab initio* LDA is based on a Fermi liquid (the electron gas), this one is based on a Luttinger liquid. First applications to inhomogeneous Hubbard models, including one containing a localized impurity, are reported.

(submitted)

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Electronic structure and magnetism of $Fe_{3-x}Cr_xSi$ alloys

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Abstract

The study of the electronic structure and magnetic properties of the $Fe_{3-x}Cr_xSi$ compound is motivated by the Mossbauer and neutron spectroscopy measurements showing unusual behaviour of Cr in such alloys. The site preferences of Cr in Fe_3Si and the effect of local environment on formation of local magnetic moments are examined using self-consistent spin-polarised TB-LMTO method. The results of calculations essentially confirm the values and orientations of magnetic moments of iron and chromium atoms. However, they do not explain an experimental observation of almost equal occupation of A, B and C sites by chromium.

(Journal of Magnetism and Magnetic Materials, 256 (2003) 46-53.

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10 Presenting Other Initiatives

10.1 CPMD Code Upgrade

CPMD Version 3.7 is now finally ready for distribution. It is a major upgrade from version 3.5.

The main improvements and changes are:

-Time Dependent DFT implementation for the calculation of excited states; Molecular Dynamics in the excited States.

-Linear Response implementation for the calculation of IR and Raman Vibrational Spectra.

-Linear Response Implementation for the calculation of NMR properties.

-Linear Scaling optimizers for the geometry optimization and transition state search.

-Direct Minimization of the Energy with k points

-OpenMP parallelization

-General Fixes

-New Manual

-Test Suite

If you have a license for CPMD 3.5, you can use the same userid/password to download the new version. Otherwise, request a new licence on-line.

10.2 Free Software Project for Atomic-Scale Computation

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It is now commonplace to say that software plays a very important role in material modeling at the atomic scale. At the same time the complexity of the methods one has to master, in many types of simulations, has grown to a level such that it is quite difficult for an individual or even a small group to start such a software project from scratch. Therefore, it appeared to us necessary to enquire about collaborative schemes that would be at the same time simple and efficient, while protecting the efforts of each individual.

The advent of rapid means of exchange of software, has helped the spread of so called "free software" or "open source" software, generally distributed under the GNU licensing scheme [1]. It is extremely effective in the computer science community (e.g. the Linux kernel development), and bioinformatics [2], and seemed to offer an interesting solution.

This scheme is still not very common in the atomic-scale simulation community, although some teams have recently started such atomic-scale "free software" projects: references [3-18] are links to softwares available under a "free software" license, or distributed without restriction on their usage (this list of softwares is not exhaustive).

On June 21-22, 2001, two of us organized a small CECAM discussion meeting on this theme. During this small meeting, we had very lively discussions, summarized in the corresponding CECAM report. Beyond the nominal theme of the meeting, many discussions evolved around recent developments in computer sciences, that have not (or little) been used by the atomic-scale simulation community.

One year later, on June 19-21, 2002, we organized a bigger CECAM meeting, as lively as the first one. Because of the larger number of participants, it seems that a critical mass was reached, large enough to launch the "free software project for atomic-scale simulations", abbreviated FSAtom.

In the present report, we will first describe briefly the notion of "free software", then, discuss in

length the possibilities of concerted code development, and finally present the FSAtom.

A. "Free software"

We will follow the nomenclature of the Free software foundation (http://www.fsf.org).

In the name "free software", the word "free" stands for freedom, not price. A "free software" is best defined by the following four basic freedoms received by the user:

- the possibility to run the program, for any purpose;

- the possibility to study how the program works, and adapt it to the needs (access to the source code is a precondition for this);

- the possibility to redistribute copies;

- the possibility to improve the program, and release improvement to the public, so that the whole community benefits (access to the source is also a precondition for this).

These four freedoms might be granted by the copyright holder to the user by different means.

Some developers do not care about copyright, and release their source code without protection (the code is in "public domain"). In this case, the freedoms are themselves not protected: everybody can modify the code, and then copyright it.

As an alternative approch, the developer can copyright his code, but distribute it under different licensing schemes. Licenses that do not give any of these four freedoms can be referred to as "proprietary". There are many intermediate licensing schemes between "proprietary" software and "free" software, a discussion of which would go beyond the aim of the present report.

Licenses also differ in the way the freedoms that they grant are protected.

The so-called "GNU General Public License" (GPL) has been central to the discussions of the above-mentioned workshops. It is chosen by more than half of all free softwares, including such important contributions as the GNU system and the Linux kernel. In the GPL, the four freedoms are protected: derivatives of GPL software have to be licensed under the GPL again, if they are being published. There is no requirement to publish modifications, but if they are being released to others, they must adhere to the GPL. This vaccinating effect against proprietarisation by third parties is often referred to as copyleft.

This license is a legal text, available at

http://www.gnu.org/copyleft/gpl.txt .

On the GNU web site, one can find more information about the license: how to use it in your program, detailed discussion of its implication, what can be done in case of violation of the license ...

B. Concerted source development

Is it possible to take advantage of the free software concept to make a concerted effort of development across different groups ?

Let us examine the present situation.

In the field of simulations at the atomic scale, many different codes coexist:

- some of them are commercialised;

- some of them are not available for sharing, except through collaboration;

- some of them are shared and can be downloaded from the Web with little constraints from the authors

On one hand, it is important that different codes are available so that cross-comparison of final results can occur, on the basis of completely independent implementations, This concept can be called "biodiversity of codes". The relationship between developpers (or developper team) is based on a (friendly) rivalry. It is the current situation. It would be easy to stay in this working mode.

However, we have to ask ourselves whether progress could be faster if more collaborative initiatives were initiated. Indeed:

- the number of codes implementing exactly the same concepts might be extremely large (e.g. in the field of electronic structure calculation based on plane waves - referred as PW codes in what follows -, there are more than a dozen of similar implementations), with a considerable loss of human time;

- accurate comparison of code results is not done on a systematic basis, or not done at all, because a protocol for doing this does not exist (one important piece of such a protocol being usually common data file formats);

- wouldn't it be more fruitful to have a few software projects, open to the community thanks to the GNU General Public License, to which anybody could contribute ?

Although the free software concept is not a prerequisite for collaborative projects, one can expect some barriers to be lowered because of the freedoms it grants.

In the CECAM discussions, it was also felt that some software projects in atomic and molecular simulations becomes so big, and the associated development so slow, that it is essential to benefit from modern software engineering concepts, like:

- libraries for handling files in view of sharing and comparison of routines and codes;

- reusability of sources;

- self-documentation of codes;

- combination of extension and compute-intensive languages (e.g. Python+C);

- high-level graphics libraries;

- installation and maintenance tools (autoconf, automake, CVS);

- self-testing of code.

These concepts are often discussed in the magazine "Computers in Science and Engineering", that has a large diffusion.

Actually, many new programming tools/languages are developed all the time and it has become

a real challenge for computational physicists to keep up with and benefit from the new developments in computer science. Establishing an organization for exchange of information among physicists about new tools/languages could therefore be of great help. Here is a list of possible topics:

- parallelism (MPI, OpenMP, ...)

- exchange of data (NetCDF, HDF, XML)

- graphics high-level libraries (VTK),

- techniques for optimisation of codes,

- use of standard libraries (BLAS , LAPACK),

- extension languages (Python, Scheme, Tkl for user interface),

- installation tools (autoconf, automake),

- maintenance tools (CVS, bug tracking),

- good coding practice (especially for big projects),

- tools for documentation (Robodoc, Src2tex, TexInfo, Docbook).

The definition of common standards is an elementary step as well. One can take the example of the development of Linux OS. In the Unix family of operating systems, the concept of "file" is central: it is the common data set that the different pieces of software treat. This fact was essential for splitting the Linux project into thousands of small subprojects.

In our field, the numerical treatment of arrays, or structured arrays is essential. Standard formats for binary files containing such structured arrays, with associated library of routines, exist: netCDF and HDF. The efficiency of routines for accessing these structures is high enough for archival and exchange use, while it is more questionable on temporary files. For text files, one might use the XML standard. One goal in our community might be to define conventions for files. Such progress can be made independently of the licensing schemes of the different codes.

The possibility of sharing pieces of software is a further step in the concerted development of codes. It might appear even without concertation between different groups, in the framework of the GNU General Public License.

At the outcome of the above-mentioned June 2002 CECAM workshop, where such ideas were discussed at length, it was decided to start the FSAtom. We reproduce below the "founding" text of the FSAtom, available on the Web site, http://www.fsatom.org . Other information are available on this Web site.

C. The FSAtom project

The Free Software Project for Atomic-scale Computation has the aim to spread the use of the "Free Software" concept in the community of Atomic-scale Computation software developers, to improve the awareness of modern software engineering concepts, and to constitute the natural place for interactions between different groups of developers in this field.

Means of action

The FSAtom project should reach this aim by taking the following actions :

* maintain a Web site (hosted by CECAM) with mailing lists and with links to the relevant software projects (also to proprietary software, for information);

* through workgroups, organize the collaboration between developers: file exchange, code testing, definition of objects, exchange of development tools, exchange of expertise ... ;

* organize workshops and tutorials on related subjects, and on modern software engineering concepts;

* maintain a contact with the Free Software foundation, and spread relevant information from it or about it;

* maintain a contact with relevant funding agencies or institutions, and ease (or foster) the writing of relevant proposals.

Organisation

During the CECAM workshop "Open Source Software for Microscopic Calculation", Lyon, 19-21 June 2002, a managing committee has been set up. For the time being, it is made of nine members:

- D. Ceperley (U. Illinois at Urbana, Urbana-Champaign, USA)
- X. Gonze (U. Catholique de Louvain, Louvain-la-Neuve, Belgium)
- K. Hinsen (Centre de Biophysique Molculaire CNRS, Orlans, France)
- K. W. Jacobsen (Tech. Univ. of Denmark, Lyngby, Denmark)
- L. Kale (U. Illinois at Urbana, Urbana-Champaign, USA)
- M. Marques (Uni. Basque Country, San Sebastin, Spain)
- G. Martyna (IBM, USA)
- D. Van Der Spoel (Uppsala U., Uppsala, Sweden)
- G. Zerah (Commissariat Energie Atomique, Bruyeres, France)

The committee has elected X. Gonze as president, and has asked CECAM to host the Web page of the project. M. Mareschal, the director of CECAM has accepted the demand, and has encouraged this project.

In the FSAtom framework, we have recently set up a Web site (hosted by CECAM, http://www.fsatom.org, Miguel Marques webmaster): mailing lists and links are a prerequisite for efficient information transfer. We have gathered a list of about sixty codes for atomic-scale simulations (with Web links), and we describe briefly those delivered under a Free software licence. We are organizing, under the auspices of CECAM, the Psi-k network and the SIMU network, a tutorial entitled "Software solutions for data exchange and code gluing", Lyon, October 8-10, 2003 (organizers : X. Gonze and K. Hinsen), followed by a CECAM workshop entitled "Component architectures, open standards, and parallel algorithms for molecular and atomistic simulations on large grids, supercomputers, workstations and clusters", Lyon, October 13-15, 2003 (organizers : G. Martyna, J. Schiotz, G. Zerah). We are also planning workgroups on selected topics (pseudopotential formats, standardized datastructures ...).

D. Conclusions

Whether these concepts will have a big impact on our community will be answered by the future. At present, everybody is welcome to register in the FSAtom mailing lists (you can find them on the fsatom Web site http://www.fsatom.org). People who deliver their software using a "free software" license are invited to send the reference URL, and a brief description of the code to Miguel Marques, marques@nautilus.fis.uc.pt or to the Webmaster of CECAM, see http://www.cecam.org . Also, developers outside a Free Software project are welcome to take part to the work group discussions.

Acknowledgments

We thank CECAM for the financial support of the two workshops, as well as for hosting the FSAtom web page.

[1] The GNU organisation, http://www.gnu.org

[2] Report about Open Source softwares in bioinformatics, http://www-smi.stanford.edu/pubs/SMI_Reports/SMI-2001-0902.pdf

[3] ABINIT, DFT code, http://www.abinit.org

[4] MMTK, Molecular Modelling ToolKit, http://starship.python.net/crew/hinsen/MMTK

[5] CAMPOS: density functional code ("dacapo"), and molecular dynamics/quasicontinuum code ("asap"), http://www.fysik.dtu.dk/campos

[6] Different softwares can be accessed from http://www.ibs.fr/ext/labos/LDM/welcome_en.htm

[7] Octopus, TD-DFT, http://www.tddft.org

[8] CP2K, Car-Parrinello 2000, http://cp2k.berlios.de

[9] PWSCF and PHONON, DFT codes, http://www.pwscf.org

[10] Gerhard Theurich's C++ DFT code, http://www.mrl.ucsb.edu/ theurich/Spinor

[11] Mondriaan, http://www.math.uu.nl/people/bisseling/Mondriaan/mondriaan.html

[12] NAMD, molecular dynamics, http://charm.cs.uiuc.edu

[13] GROMACS, molecular dynamics, http://www.gromacs.org

[14] PyMOL, molecular visualisation, http://pymol.sourceforge.net

[15] Digital materials, http://www.tc.cornell.edu/Research/Multiscale

[16] PWPAW, DFT code, http://www.wfu.edu/ natalie/papers/pwpaw/man.html

[17] CPW2000 pseudopotential code, http://bohr.inesc.pt/ jlm/pseudo.html

[18] FPMD, http://www.cineca.it/ acv0/CP/carpar.html

11 SCIENTIFIC HIGHLIGHT OF THE MONTH

Electric transport perpendicular to the planes

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Abstract

Since the discovery of the giant magnetoresistance (GMR) in magnetic multilayers several theoretical descriptions have been used to determine the resistivity of such a layered structure. Though the resistance for the current in direction of the planes of layers can easily be measured and has been intensively studied in theoretical works [1, 2], the GMR for the current perpendicular geometry (CPP) is slightly more difficult to describe. Here, a formalism for the investigation of the CPP GMR is reported by making use of the Kubo-Greenwood equation. This formalism is a useful tool for the discussion of the influence of the interfaces on the GMR. The presentation of the Kubo-Greenwood formalism for CPP transport is complemented by a brief discussion of some results.

1 Introduction

The behavior of two magnetic layers separated by a nonmagnetic material strongly depends on the magnetic configuration of the two magnets. Usually the resistance of the system drops down if a magnetic field is applied and, therefore, the magnetic moments of the two magnets are parallel aligned. This effect is known as giant magnetoresistance (GMR) and has been intensively studied during the last fifteen years [3, 4]. The above described GMR is somehow different from the *natural* magnetoresistance effect (anisotropic magnetoresistance = AMR, Hall effect). The AMR, can be observed in every metal due to the Lorentz force on the conduction electrons and depends on the angle between the magnetization and the current [5, 6]. This magnetoresistance

is caused by the fact that the magnetization in thin films is not homogenous, but is influenced by domain walls and other impurities, which means the resistance measured parallel to the magnetization direction is different from the resistance perpendicular to the magnetization direction of the film. It has been tried to use the AMR for technical purposes, but the applications were restricted to low temperatures.

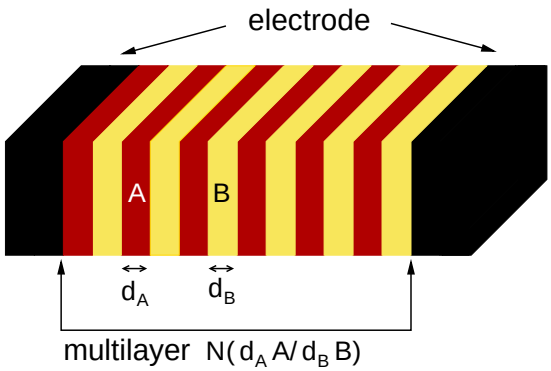

Figure 1: Schematic drawing of a multilayered structure, which consists of alternating layers of material A and B. The thickness of the layers is denoted by d_A and d_B. The multilayer is covered by two magnetic leads (electrodes).

The situation started to change, when Baibich and others observed the GMR effect in sandwich structures, Fe/Cr/Fe in particular. Similar trilayered structures have been already used to examine the tunneling magnetoresistance in FM/SC/FM (SC = semiconductor) sandwiches so called tunnel junctions [7, 8]. The GMR has the advantage that it is usually larger than the AMR and is suitable for measurements at elevated temperatures [9]. In contrast to the AMR the GMR occurs only in systems in which an external magnetic field can change the magnetic configuration of the system or in other words the coupling between the layers is not too strong or even FM. However, for practical purposes the GMR of a single FM/NM/FM trilayer (FM = ferromagnetic, NM = nonmagnetic) is still too small, but it has been observed that the effect can be increased by using more complex multilayer structures (Fig. 1).

The fact that the magnetic configuration in such materials can easily be switched by a magnetic field makes them interesting for technological applications. Several fabrication techniques have been developed in the past, which allow to built high quality superlattices, multilayers or spin-valves [4]. These systems can generally divided in two classes: coupled and non-coupled systems. In coupled structures the magnetic configuration of both magnets is influenced by the external field, whereas in non-coupled (e.g. spin-valve) systems the magnetic configuration of one FM is kept fixed by an additional anti-ferromagnetic (AF) layer [10]. Today, the GMR is already used in reading heads of CD disc drives and for magnetic data storing – MRAM technology [11, 12]. It should be mentioned that for technical purposes often systems with semi-conducting spacers are used, which means making use of the TMR effect.

As mentioned above the GMR is caused by a magnetic field, which changes the scattering of the conduction electrons [6]. However, the electric transport properties of multilayers are also influenced by the preparation technique, temperature etc. [13]. These effects determine the

structure of the interface, e.g. the occurrence of interdiffusion and alloy formation. Furthermore, the GMR depends on the thickness of the NM and FM layers. Closely related to these topics is the question of the interlayer exchange coupling (IEC) in such systems, because it has been shown that AF coupling supports the possibility of spin-dependent transport and gives possibilities for practical applications [14].

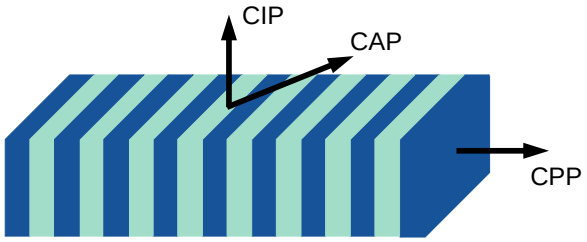

Figure 2: Different geometries are possible for GMR studies. Mainly two configurations are used: current perpendicular to the planes (CPP) and current in plane (CIP) geometry. In general the current has a certain angle to the planes (CAP).

Besides the above mentioned features, the size of the GMR in a layered structure also depends on the experimental setup. The easiest way to measure a resistance in a multilayer is for current in plane (CIP) geometry, see Fig. 2. The CIP GMR can be quite large. Unfortunately, the CIP resistance is not very interesting for technical applications, because the important features of a multilayer occur in growth direction. In addition, measurements in CIP geometry are not sufficient to determine the current density [15]. In contrast to that measurements with the current perpendicular to the planes (CPP) give very accurate results. Though, measurements in CPP geometry are much more complicated as compared to CIP experiments [4, 16] the CPP GMR may be important for applicational purposes at low temperatures ($\leq T_{\mathrm{room}}$), because it is large as compared to the CIP MR [16, 17].

Today, several preparation techniques exist making use of the CPP GMR and related phenomena in magnetic multilayers, see Ref. [16, 18]. Nonetheless, there is still no real consense what the main cause of the GMR is: the connection between the electronic band-structure and the magnetic moments of the layers or the spin-dependence of the single-site scattering potentials [19]. Besides that there exists a number of more practical questions, which depend on the particular system, e.g. how does interdiffusion influences the size of the GMR and how are the GMR and IEC related? The calculational approaches used to investigate the resistances range from the semi-classical Boltzmann theory [5] to quantum-mechanical descriptions, e.g. the Kubo-Greenwood equation [19, 20, 21]. A third method intensively used for the examination of ballistic transport in tunnel-junctions is the Landauer-Büttiker method. This method describes transport properties on a mesoscopic scale, which means that the results depend on the size of the sample. The resistances are measured far away from the FM/NM interfaces. Therefore, a description of effects near the interfaces is somewhat difficult to include. However, the structure of the interface can be described quite easily within the Kubo-Greenwood approach. Alloy formation, impurities and other effects can be included in the calculation. This may be important for the comparison with the measurements and the interpretation of the experimental findings.

A detailed description of the Kubo-Greenwood equation and its application to layered structures is presented in Sec. 3. Before that, in Sec. 2 an overview of relevant experimental results and technique is given. Finally, some results concerning CPP transport in Fe/Cr/Fe and Fe/Si/Fe sandwiches will be discussed in Sec. 4.

2 CPP transport from the experimental point of view

In this section some fundamental experimental results concerning GMR effect and related properties are presented. Results for the TMR are not shown. The GMR effect can be measured between a FM and any disordered magnetic state of the multilayer. Usually the GMR ratio is defined as the change of the resistance under a magnetic field **H** (FM solution) relative to the resistance of the zero field state R^0

$$R^{\exp} = \frac{R^0 - R^H}{R^0}. \tag{1}$$

Today, some authors use the saturation state instead of the zero field state, because in this case the contribution from spin disorder is minimized [6]. In theoretical calculations it is convenient to assume that the zero field state corresponds to a perfect AF arrangement of the magnetic moments of the leads, where effects of spin disorder etc. are neglected. The GMR is then given by the difference between the parallel (FM) and antiparallel (AF) solution, whereby R^0 is replaced by R^{FM}

$$R = \frac{R^{\mathrm{FM}} - R^{\mathrm{AF}}}{R^{\mathrm{AF}}}, \quad R \leq 1. \tag{2}$$

Here, the difference of the resistances is divided by the anti-ferromagnetic configuration R^{AF}, which gives a bounded solution provided that $R^{\mathrm{AF}} > R^{\mathrm{FM}}$. It is also common to use an unbounded solution dividing by R^{FM} instead of R^{AF}.

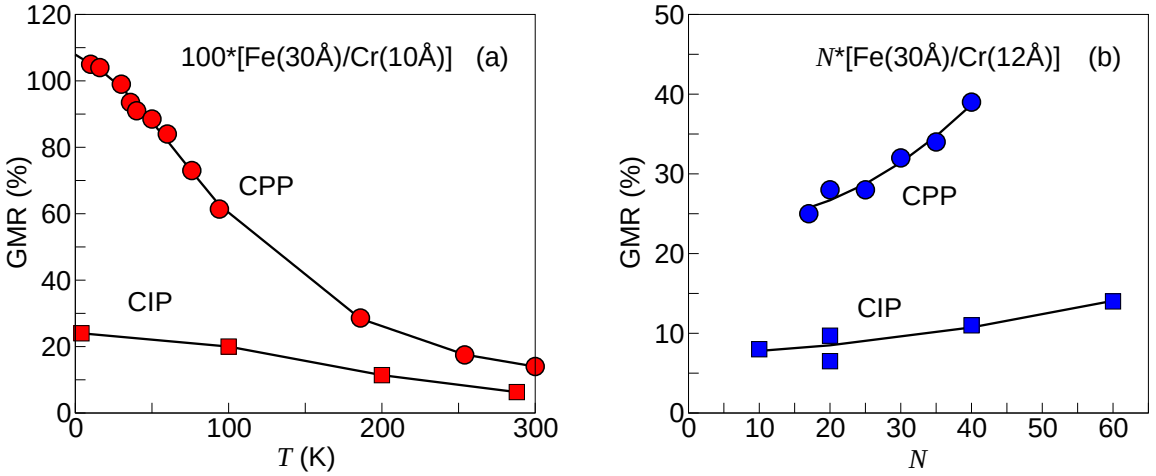

Figure 3: Measured GMR of Fe/Cr multilayers at varying temperatures (a) and depending on the number of bilayers N (b). The experimental data are taken from the Refs. [16] and [22].

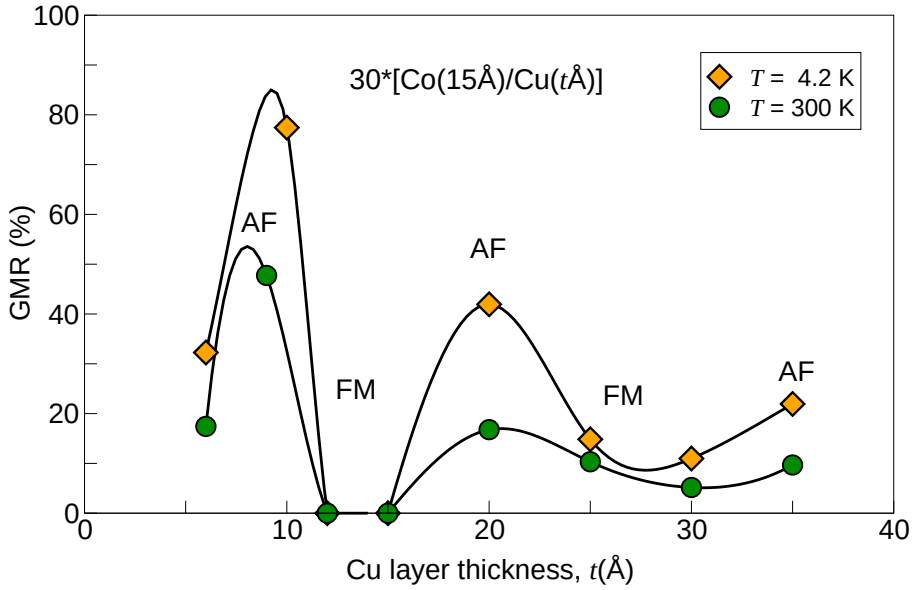

Figure 4: Measured GMR of Co/Cu multilayers with varying thickness of the Cu layers t. The oscillations can be related to the oscillations of the interlayer exchange coupling of the Co layers. The data are taken from Ref. [23].

Some typical experimental results for the GMR of the most famous multilayers: Fe/Cr and Co/Cu, are reproduced in the Figs. 3 and 4. It is known that the size of the GMR depends on the temperature (Fig. 3a). At low temperatures the CPP GMR is much larger as compared to the GMR measured in CIP geometry, which was predicted before by several theoretical investigations [24, 25]. With increasing temperature the difference between CIP and CPP GMR becomes smaller and in some cases the CIP GMR may become larger than the CPP one [16]. In addition, the GMR of a multilayered structure depends on the number of bilayers, e.g. repetition of the two components (Fig. 3b). In the case of Fe/Cr it has been observed that the size of the CPP GMR strongly increases with growing number of repetitions N, whereas the CIP GMR is not much effected by N (Fig. 3b). Furthermore, the GMR of a Co/Cu multilayer is shown in Fig. 4 depending on the thickness of the NM Cu layer. The size of the GMR strongly oscillates with the thickness of the Cu layer. It has been shown that these oscillations are related to the interlayer exchange coupling of the two leads [3].

3 Electric transport within the Kubo-Greenwood formalism

3.1 Kubo-Greenwood equation

In order to determine the resistance of a layered system described in the previous section we can make use of Kubo's method [20]. The Kubo formula describes the response of a quantum mechanical system to an external field, e.g. the change of the electric current due to an electric field, whereby it is assumed that the perturbation is small and therefore the relation between

field and current can be assumed to be linear. In this case the Hamiltonian of the original system is modified by a perturbation $\widehat{\mathbf{H}}'$

$$\widehat{\mathbf{H}} = \widehat{\mathbf{H}}_\mathbf{0} + \widehat{\mathbf{H}}', \tag{3}$$

where $\widehat{\mathbf{H}}_\mathbf{0}$ describes the unperturbated system. Here, the perturbation is chosen to be

$$\widehat{\mathbf{H}}' = -\mathbf{pE} \tag{4}$$

assuming that the electric field $\mathbf{E}$ is a periodic quantity and $\mathbf{p}$ the electric dipole-moment

$$\mathbf{E} = \mathcal{E} e^{-i(\omega+i\delta)t}. \tag{5}$$

The present choice of $\mathbf{E}$ ensures that the perturbation vanishes for $t = -\infty$ if $\delta \to 0$. In linear response the electric current is related to the electric field by the two-point conductivity tensor $\underline{\underline{\sigma}}(\mathbf{r}, \mathbf{r}')$

$$\mathbf{j}(\mathbf{r}) = \int d^3r' \underline{\underline{\sigma}}(\mathbf{r}, \mathbf{r}')\mathbf{E}(\mathbf{r}'). \tag{6}$$

In the limit of static, homogeneous electric fields, i.e. in the zero frequency limit, the Kubo approach yields for the conductivity [20, 26, 27]

$$\underline{\underline{\sigma}}(\mathbf{r}, \mathbf{r}') = -\lim_{\omega\to 0} \frac{1}{\omega} \underline{\underline{\Pi}}(\mathbf{r}, \mathbf{r}', \omega) \tag{7}$$

with $\Pi(\mathbf{r}, \mathbf{r}', \omega)$ being the current-current correlation function

$$\underline{\underline{\Pi}}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{V} \int_0^\infty d\tau e^{i\omega\tau} \langle \left[\widehat{\mathbf{j}}(\mathbf{r}, t+\tau), \widehat{\mathbf{j}}(\mathbf{r}', t)\right] \rangle, \tag{8}$$

in which V denotes the unit volume. Here, $\langle \quad \rangle$ denotes the expectation value over all states of the system at zero temperatures and $\widehat{\mathbf{j}}(\mathbf{r}, t)$ is the quantum mechanical current operator

$$\widehat{\mathbf{j}}(\mathbf{r}, t) = e^{i\widehat{H}_0 t} \widehat{\mathbf{j}}(\mathbf{r}) e^{-i\widehat{H}_0 t}, \qquad \widehat{\mathbf{j}}(\mathbf{r}) = \frac{e\hbar}{mi} \psi^\dagger(\mathbf{r}) \underline{\nabla_r} \psi(\mathbf{r}). \tag{9}$$

Finally, Eq. (8) leads to the Kubo-Greenwood equation for the electric conductivity

$$\sigma_{\mu\nu} = \frac{\pi\hbar}{V} \langle \sum_{mn} j^\mu_{mn} j^\nu_{nm} \delta(\epsilon_\mathrm{F} - \epsilon_m) \delta(\epsilon_\mathrm{F} - \epsilon_n) \rangle, \tag{10}$$

with μ and ν denoting the Cartesian indices x, y, z [20, 26]. The expression in Eq. (9) holds only for nonmagnetic metals. However, at least the lead material of a multilayer is magnetic, which leads to charge and spin accumulation effects. This problem can be overcome by introducing spin-dependent current densities, see for example Refs. [21, 28].

3.2 Application to layered structures

The general expressions discussed in Sec. 3.1 can be simplified assuming a layered structure which provides two-dimensional translational symmetry. Suppose the layers grow along the z-axis and the fields in the $(x-y)$-plane are homogeneous then Eq. (6) reduces to

$$\mathbf{j}(z) = \int dz' \underline{\underline{\sigma}}(z, z')\mathbf{E}(z') \tag{11}$$

Usually transport measurements are carried out for current in the $(x-y)$-plane (CIP) or perpendicular to the plane (CPP) geometry, compare Fig. 2. For fields in the CIP case the calculation of the $\underline{\underline{\sigma}}(z,z')$ matrix is straight forward, because the electric field in z-direction is constant. This leads to

$$j(z) \;=\; E \int dz' \underline{\underline{\sigma_{\parallel}}}(z,z'). \tag{12}$$

Until now the current is still a microscopic quantity. The measured current corresponds to the expectation value of the current divided by the system size, i.e. length of the system in growth direction L

$$\langle j(z) \rangle \;=\; E \frac{1}{L} \int dz dz' \sigma_{\parallel}(z,z') \;=\; E\,\sigma_{\mathrm{CIP}}. \tag{13}$$

The situation becomes more complex if we apply the electric field perpendicular to the planes. In this case the electric field $E(z)$ is no longer constant. However, it will be shown that the transport in CPP geometry can be handled similarly to the CIP case assuming steady state conditions [6]. In order to discuss perpendicular transport it is more convenient to use the inverse of Eq. (11)

$$E(z) \;=\; \int dz' \rho_{\perp}(z,z') j(z'). \tag{14}$$

In the steady state the electronic density is time-independent, i.e. $\partial\rho/\partial t = 0$. Due to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \mathbf{j} = \frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial z} \;=\; 0 \tag{15}$$

it follows that Eq. (15) is fulfilled only if the current is constant. In this case Eq. (14) can be rewritten

$$E(z) \;=\; j \int dz' \rho_{\perp}(z,z'). \tag{16}$$

The microscopic quantities in Eq. (16) can now be used to express the measured electric field, which is at least the average divided by the system size L

$$\langle E \rangle \;=\; j \frac{1}{L} \int dz dz' \rho_{\perp}(z,z') \;=\; j\,\rho_{\mathrm{CPP}}, \tag{17}$$

where ρ_{CPP} corresponds the measured resistivity.

The last step is to determine the resistivity or sheet resistance (see next section) of a layered system. However, from the Kubo-Greenwood formula Eq. (10) the conductivity is known, therefore one has to solve the following integral equation to obtain the resistivity ρ_{CPP} Eq. (17) of the system

$$\int dz'' \sigma_{\perp}(z,z'') \rho_{\perp}(z'',z') \;=\; \delta(z-z'), \tag{18}$$

which means inverting the conductivity matrix

$$\rho_{\perp}(z,z') \;=\; \sigma_{\perp}^{-1}(z,z'). \tag{19}$$

3.3 Sheet resistance

In our calculations we use the so called sheet resistance being the product of the resistivity and the system length

$$r = L\rho_{\mathrm{CPP}} = \int dz dz' \rho_{\perp}(z, z'), \tag{20}$$

where z and z' are still continuous variables perpendicular to the planes. The purpose of the following transformation is to map the conductivity tensor $\sigma(z, z')$ on a discrete expression for layered systems σ_{pq}^{zz}, with p and q denoting planes of atoms

$$\sigma(z, z') \longrightarrow \sigma_{pq}^{zz'}(n), \tag{21}$$

whereby n is the total number of layers taken into account. Due to the symmetry of the problem the mapping concerns only the z-components and the index z is suppressed in the following discussion. The mapping should conserve the formal structure of the problem such that yields

$$\int dz'' \sigma(z, z'')\rho(z'', z') = \delta(z - z') \longrightarrow \sum \sigma_{pr}(n)\rho_{rq}(n) = \delta_{pq}. \tag{22}$$

The necessary condition for the transformation in Eq. (22) is that the Cauchy convergence criterion is fulfilled. Here, the Cauchy criterion corresponds to

$$\left| r - \lim_{n\to\infty} r(n) \right| < \epsilon, \quad n \in N^{+}, \tag{23}$$

with ϵ being an infinitesimal small number. In this case the integral in Eq. (20) can be replaced by the sum over the planes of atoms

$$r(n) = \sum_{p,q=1}^{n} \rho_{pq}(n). \tag{24}$$

If the above mentioned conditions are fulfilled Eq. (24) can be used to calculate the sheet resistance of a layered system in CPP geometry. However, it should be kept in mind that the actual quantity, which is interesting in electric transport, is the change of the resistance due to an applied magnetic field, see Sec. 1. Therefore, it has to be taken into account that the sheet resistance also depends on the magnetic configuration of the leads $\mathcal{C}$. The two configurations considered in the calculations are displayed in Fig. 3. Therein, the leads used to be semi-infinite systems, i.e. bulk potentials or vacuum, which cover the spacer layers [19].

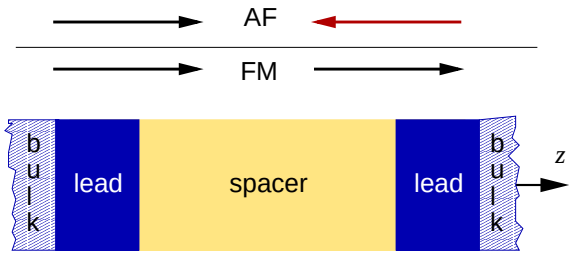

Figure 5: Schematic drawing of a trilayer. The NM spacer is covered by two semi-infinite FM leads (bulk), whereby some additional lead layers are used as buffer layers in the selfconsistent calculation (dark part). The two magnetic configurations used for the calculation of the GMR are marked by the arrows.

The FM configuration agrees with the experimental solution for an applied magnetic field and the AF case corresponds to the zero field situation, see Sec. 2. Due to technical reasons, i.e.

k-space integration and the handling of the surface Green's function it is helpful to evaluate the Kubo-Greenwood equation for a small but finite imaginary part of the Fermi energy $\epsilon_F - i\delta$. The actual sheet resistance for $\delta \to 0$ is then determined by

$$r(\mathcal{C}, n) \;=\; \lim_{\delta \to 0} r(\mathcal{C}, n, \delta) \;=\; \lim_{\delta \to 0} \sum_{p,q=1}^{n} \rho_{pq}(\mathcal{C}, n, \delta). \tag{25}$$

Accordingly, using the definition in Eq. (2) the CPP magnetoresistance within the Kubo-Greenwood formalism is given by

$$R(n) \;=\; \frac{r(\mathrm{AF}, n) - r(\mathrm{FM}, n)}{r(\mathrm{AF}, n)}. \tag{26}$$

In addition to Eq. (25) a layer-resolved sheet resistance can be defined by

$$r_p(\mathcal{C}, n) \;=\; \sum_{q=1}^{n} \rho_q(\mathcal{C}, n). \tag{27}$$

This expression can be used for a detailed discussion of the origin of the resistance, see Sec. 4.

Two problems arise from the above definition Eq. (26). First, charge and spin accumulation effects, which occur at the lead-spacer interface, require that a particular number of lead layers is included in the selfconsistently calculated part of the multilayer (dark regions in Fig. 5). It can be shown that for a sufficient large number of lead layers and a given value of δ the sheet resistance varies linear with n. For $\delta \to 0$ the sheet resistance is then independent from the number of lead layers, for details see Ref. [29]. A typical example is displayed in Fig. 6a for a $Fe_{12}/Si_9/Fe_{12}$ trilayer and $\delta = 2\,\mathrm{mRy}$.

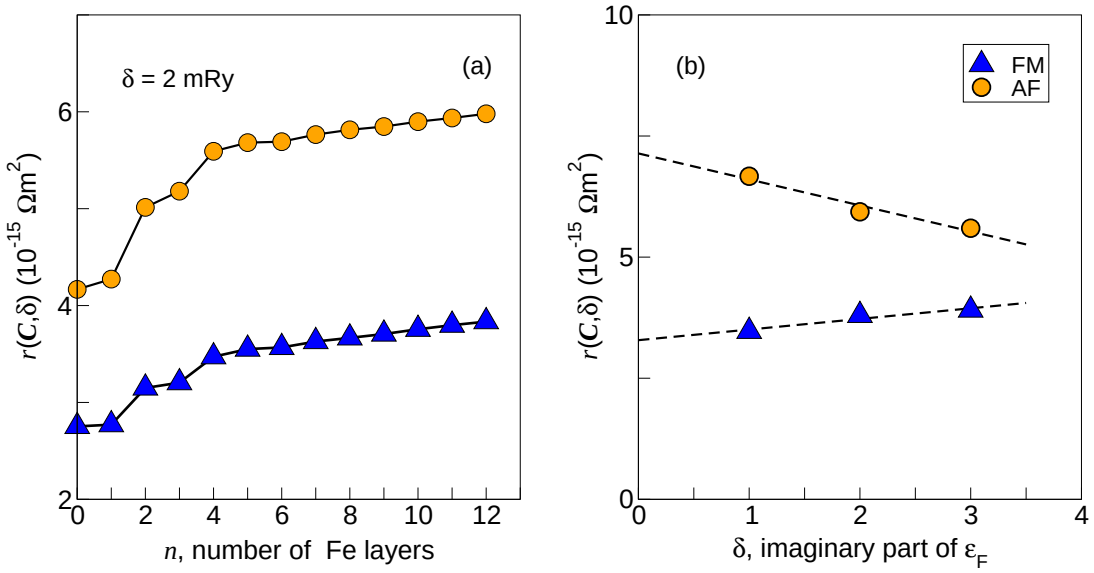

Figure 6: Variation of the sheet resistance $r(C, n, \delta)$ with the number of Fe lead layers n (a) and with the imaginary part of the Fermi energy δ (b) for a $Fe_{12}Si_{12}Fe_{12}$ trilayer. In both cases the results are shown for the AF (triangles) and FM (circles) alignment of the leads.

Second, from Eq. (25) it is obvious that the sheet resistance depends on the imaginary part of the Fermi energy. However, the sheet resistance varies linearly with δ provided the number of buffer (lead) layers is large enough, see Fig. 6b. Therefore, the actual sheet resistance can be obtained from calculations for finite δ [29].

4 Some results

In this section some numerical applications of the approach for CPP transport in layered structures (see Sec. 3.2) will be presented. All numerical input, which is necessary for the calculation of the sheet resistance Eq. (24), has been obtained from the fully-relativistic spin-polarized version of the screened Korringa-Kohn-Rostoker (SKKR) method [30, 31]. Technical details concerning the calculation of the electronic and magnetic properties can be found in Refs. [29, 32].

Basically the GMR is calculated for different spacer thicknesses, i.e. different numbers of NM layers, compare Fig. 5. A typical result of the GMR is displayed in Fig. 7a for a Fe/Cr/Fe trilayer. The GMR is plotted versus the number of Cr layers, whereby the Cr thickness ranges from 2 ML to 42 ML. With increasing number of Cr layers the GMR decreases from 28 % to $\approx 5\,\%$. However, the decrease is accompanied by oscillations, which depend on the number of Cr layers. In order to show that the oscillations are related to the interlayer exchange coupling (IEC) the energy difference between the two magnetic

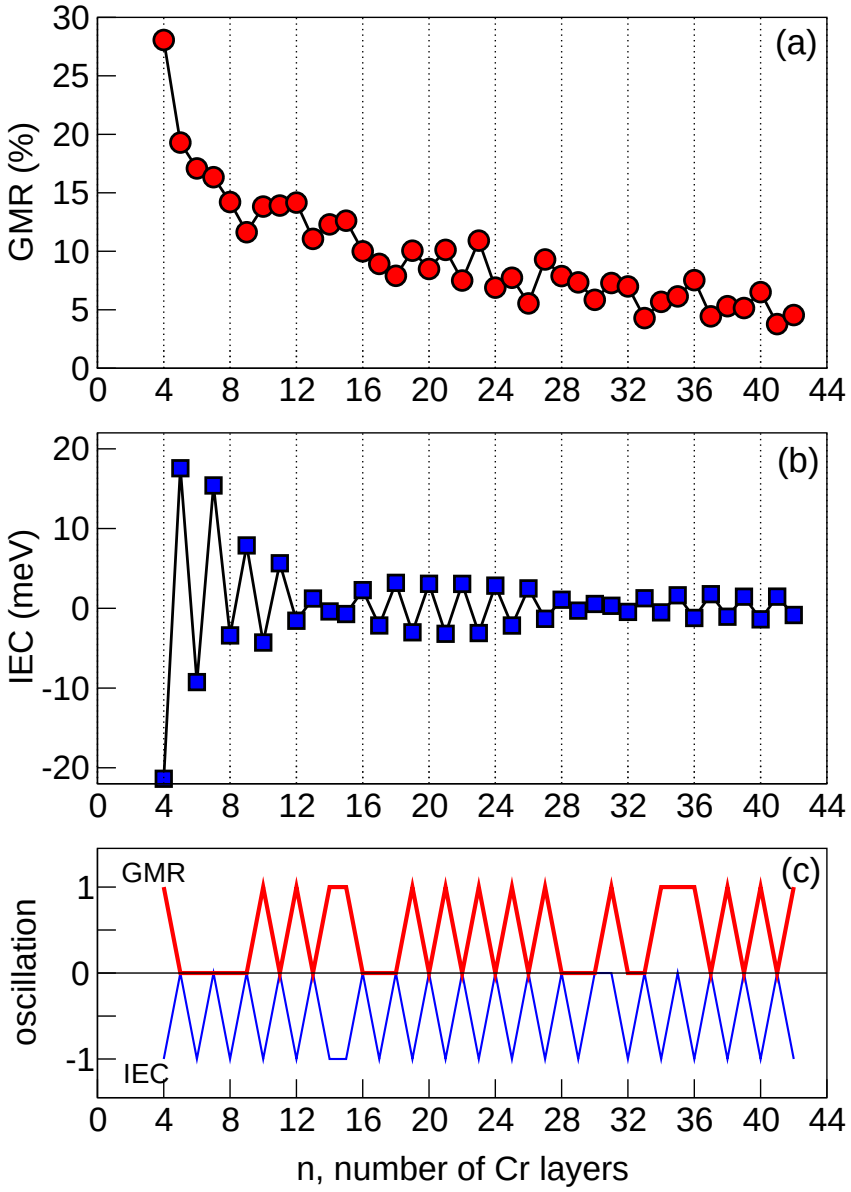

Figure 7: (a) The GMR of Fe/Cr/Fe trilayers depending on the number of Cr layers n. (b) Interlayer exchange coupling (IEC) for Fe/Cr/Fe obtained from the band energy difference vs. the number of spacer layers n. (c) Comparison of the oscillations of the GMR and the IEC of the above shown trilayers, for details see text. Data are taken from Ref. [33].

states $\Delta E = E(\mathrm{AF}) - E(\mathrm{FM})$ has to be examined. In here, the IEC has been obtained by applying the magnetic force theorem [30, 32]. The results are given in Fig. 7b. The oscillations of the GMR and IEC have been compared by checking whether the GMR(n) < GMR(n+1) or vice versa. In the first case the value of the oscillation for the (n+1)-layer system is set to one, whereas in the second case it is chosen to be zero. A similar procedure has been used for the IEC choosing zero for AF coupling and -1 for FM coupling, respectively. The results are summarized in Fig. 7c. From this viewgraph it is obvious that the two ML period of the IEC can be observed in the GMR. In addition, the phase slips occurring every 15-16 ML also exist,

but they are slightly shifted and smeared out. In this system the local minima in the GMR correspond to FM coupling and the maxima to AF coupling, respectively.

Furthermore, this method can also be used to examine systems with some configurational disorder, which may occur at the interfaces by interdiffusion. The disorder is described within the coherent potential approximation (CPA). That the CPA concept is sufficient for layered systems was shown in a previous paper [19]. An example for a system in which interdiffusion effects are important is Fe/Si. This system tends to build CsCl-like FeSi alloys near the interfaces [34]. In our calculations we have assumed that the interdiffusion region is restricted to the direct interface [32]

$$\ldots \mathrm{Fe/Fe}_{1-c_\mathrm{d}}\mathrm{Si}_{c_\mathrm{d}}/\mathrm{Fe}_{c_\mathrm{d}}\mathrm{Si}_{1-c_\mathrm{d}}/\mathrm{Si}_{s-2}/\mathrm{Fe}_{c_\mathrm{d}}\mathrm{Si}_{1-c_\mathrm{d}}/\mathrm{Fe}_{1-c_\mathrm{d}}\mathrm{Si}_{c_\mathrm{d}}/\mathrm{Fe}\ldots$$

The GMR obtained from Eq. (2) for different interdiffusion concentrations c_d is shown in Fig. 8. The calculations have been performed for three particular systems with 6, 9, and 12 ML of Si taking into account a two-layer interdiffusion. For $c_\mathrm{d} = 0$ the GMR is extremely large (50 %), which has not been reported in any experiment. However, independently from the number of spacer layers the GMR immediately breaks down if alloy formation takes place at the interfaces (Fig. 8).

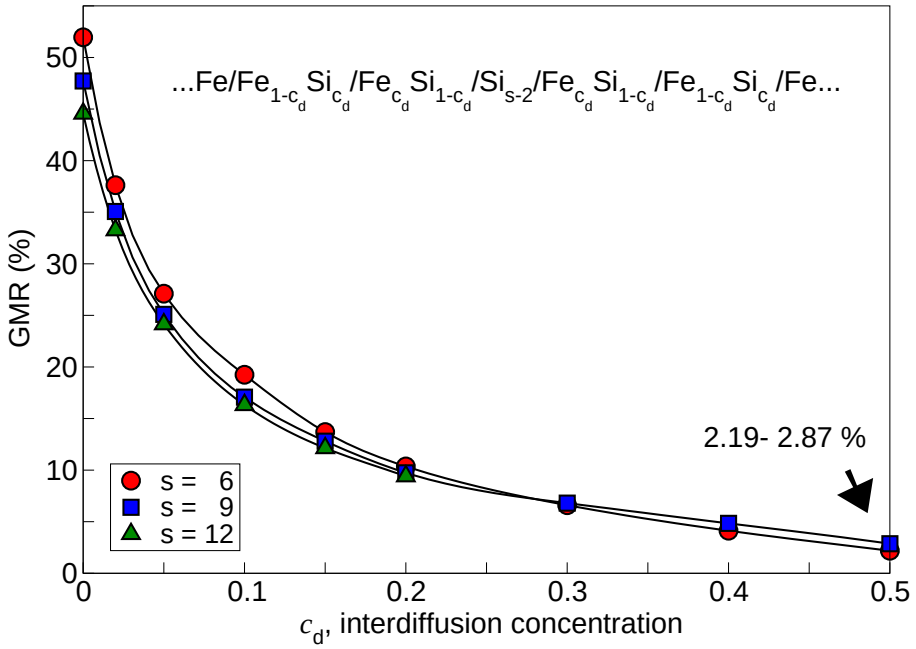

Fig. 8: GMR for Fe/Si$_s$/Fe trilayers vs. the interdiffusion concentration c_d for different spacer thicknesses s. Data are taken from Ref. [32]

If the interdiffusion reaches 20 % the GMR is already reduced to a fifth of the value for $c_\mathrm{d} = 0$. It is known from the literature that a $\mathrm{Si}_{0.5}\mathrm{Fe}_{0.5}$ alloy is quite likely to occur at the Fe/Si interfaces [34, 35]. The GMR of Fe/Si systems lie below 2.2 % [36, 37]. The present calculation for $c_\mathrm{d} = 0.5$ (Fig. 8) are in a good agreement with the experimental findings, which allow the conclusion that the small GMR of Fe/Si multi- or trilayers is strongly related to the formation

of Fe/Si alloys at the interfaces.

The GMR obtained from Eq. (2) and Eq. (24) provides only information for the whole trilayer. In order to check which layers or parts contribute mostly to the GMR it is helpful to use sheet resistance fractions. These fractions can be obtained from Eq. (27) by investigating the differences of the layer-resolved sheet resistances for the leads (region I and V), the spacer (III), and the interfaces (II and IV). An example is shown in Fig. 9 for the $Fe_{12}/Si_6/Fe_{12}$ system. From this figure it is obvious that the main contribution stems from the interfaces. In the case of $c_d = 0$ there still exists a reasonable large contribution (20 %) from the spacer. With increasing interdiffusion the latter one becomes smaller and vanishes at least for $c_{\mathrm{d}} = 0.2$. The contributions from the leads are negligible.

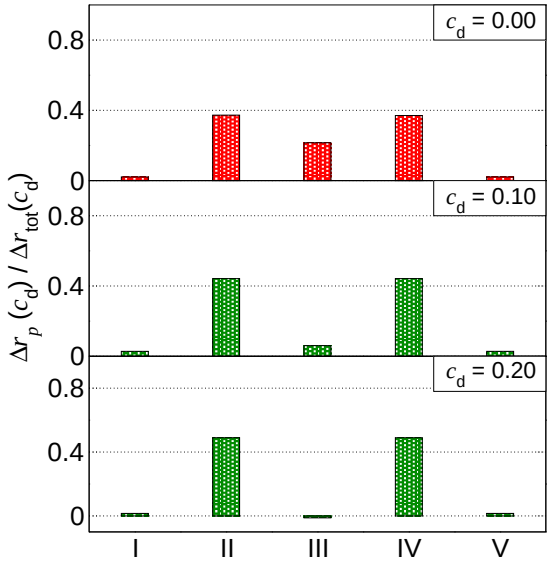

Figure 9: Normalized fractions of the layer-resolved sheet resistance differences Δr_p for characteristic regions p of $Fe_{12}/Si_6/Fe_{12}$. In the upper panel the results for the system with ideal interfaces are shown. The results for interface alloying are displayed in the middle and bottom panel. Roman numbers mark particular regions of the system: I left lead, II left interface, III spacer, IV right interface, and V right lead.

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