Ψ_k Newsletter

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

Number 54 December 2002

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Contents

1 Editorial

We start this newsletter with a call for abstracts of newly submitted papers. Please do read this and try to respond positively because the success of this section depends solely on your contributions. The section **News from RTN1 ("Magnetoelectronics")** network contains detailed report, including abstracts of presented papers, on its second annual meeting and mid-term review. In the same section we have an announcement of this network's workshop on "Spin Mesoscopics". In the **News from the RTN2 and RTN3 ("f-electrons" and "Exciting")** networks section readers will find a few postdoctoral position announcements, and an announcement of the first hands on workshop of the RTN2 ("f-electrons") workshop entitled "Workshop Hands-on-FPLO". This workshop will take place in Dresden on March 28-April 1, 2003. The **News from the ESF Programme** section contains four elaborate reports on the ESF supported workshops. All of them include abstracts of presented papers. The Hands-on VASP Code Workshop is also announced here. In the **Genaral Workshop/Conference Announcements** section there are a number of announcements of other future workshops and meetings. More position announcements can be found in the **General Job Announcments** section. As always, the abstracts of newly submitted papers are placed in the usual **Abstracts** section. In the **Book Announcements** section Peter Mohn (*Vienna, Austria*) announces his book on the **"Magnetism in the Solid State, An Introduction"**. Following the latter is a call for nominations for the Michelson Postdoctoral Prize Lectureship at the Case Western Reserve University. The newsletter is finished with the scientific highlight of the month by Stephen Fahy, Paul Delaney, and Jim Greer (*Cork, Ireland*) on **"Pseudo-interactions and the electron-electron cusp"**. Please see the table of contents for further details.

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

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

The above contains information on the Psi-k 2002 workshops and hands-on courses. 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 Call for Abstracts of Newly Submitted Papers

We have noticed a sharp decline in submissions of abstracts to the Psi-k newsletters. The purpose of the **Abstracts** section is to keep the whole Psi-k community aware of our common interests and research efforts at any particular time, and to stimulate more collaboration and enhance collaborative visits between scientific institutions across Europe. So, we would like to encourage all of you to send us your abstracts. The abstract template is attached below. If you feel however that it takes too much of your time to fill in the template, then just extract your abstract from your article and send it to us anyway. Do not wait until your paper is accepted or published, because it misses the point of the **Abstracts** section.

It seems that all of us make an effort to send our manuscripts to the Los Alamos cond-mat database which is much broader than our ab initio field. However, our **Abstracts** section is much more focussed subject-wise and could give us faster access to the relevant information.

Thank you for your consideration.

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3 News from the RTN1 ("Magnetoelectronics")

COMPUTATIONAL MAGNETOELECTRONICS

3.1 Reports on RTN1 Workshops/Meetings

3.1.1 Report on 2nd Annual Meeting and Mid-Term Review

CNRS, Oléron Island, France

October 5-9, 2002

The second annual meeting of the RT-Network, which took place in a CNRS-center on Oléron Island (France) from October 5-9, 2002, was organized by the French node, Frédéric Petroff in particular. This meeting consisted of three parts: the annual meeting of the Research Training Network with a number of review lectures presenting new developments in the network, the mid-term review with R. Monk from the EU in Bruxelles, and following that a symposium on magnetic semiconductors and half-metallic systems. Over eighty members of the ten national nodes participated to the 2nd annual meeting discussing and reviewing the activities of the network and more than half of the participants were able to join the subsequent symposium on magnetic semiconductors and half metalic systems. Three external speakers were invited to the symposium – Tomasz Dietl (Warsaw), Thomas Schulthess (Oak Ridge), and Hiroshi Katayama-Yoshida (Osaka) – who are leading experts on the magnetic semiconductors and half metalic systems.

2nd annual meeting:

The meeting started with twelve lectures and review talks given by the node members presenting the activities of the different nodes and the progress which has been made during the last year. A central issue was the study of spin-dependent transport phenomena. The investigated systems and topics reached from electronic transport in nano-wires, which are promising candidates for spin filters, to giant magnetoresistance (GMR) studies of realistic spin-valve systems. Some lectures focussed on spectroscopic studies of FM/SC/FM (FM = ferromagnet, SC = semiconductor) trilayers or heterostructures and the role of spin torques in magnetic multilayers. The methods covered quantum-mechanical just as semi-classical approaches. Furthermore, three talks were devoted to related topics concerning the electronic and the magnetic structure of FM/SC interfaces and half-metallic systems. The relevance of proximity effects in

FM/superconductor structures was discussed in another talk. The series of lectures was completed by two experimental talks on spin-polarized transport in FM/SC heterostructures and tunneling in half-metallic manganite systems.
In order to give the opportunity for further discussions a poster session was organized for the first time. The poster sessions were highly frequented and they were starting point for many intense discussions during the annual meeting. This possibility for lively exchange was used in particular by the young PhD-students and post-docs of the Network.
As can be seen from the above reviews and the enclosed abstracts, research in the Network does not only cover different properties of spin-transport, but is complemented by related topics. It turned out, that the collaboration between the nodes has been strengthened during the last year and all post-doc positions are occupied.

Mid-term review

The second part of the meeting started on Monday afternoon with the talks of the young Network researchers whereby every presentation consisted of two parts. During the first part the PhD-students and young post-docs had the opportunity to present their work and discuss their results, while in the second, shorter, part they should report on their experiences in the Network including practical matters like settling in a new environment and their integration in the team. All young researchers seemed to feel accepted in the groups of the Network. Some of them underlined that collaboration with other groups of the Network was very fruitful. However, it was criticized that the Network gives no long-term perspectives.
The scientific talks picked up and consolidated interesting aspects of the lectures given during the 2nd annual meeting. Spin-dependent transport was discussed in the framework of the Kubo-Landauer and the Kubo-Greenwood method, whereby spin-injection in Fe/InAs and calculations of tunneling spectroscopy were discussed. Besides that transport properties of Co/Cu systems with Cr impurities, and the influence of interdiffusion on Fe/Si/Fe trilayers was discussed. Andreev bound states and spontaneous current in FM/superconductor heterostructures have been investigated by solving the Hartree-Fock-Gorkov equations. Furthermore, two talks were devoted to half-metallic systems, in which tunneling in LSMO junctions was discussed and a new group of half-metals consisting of $3d$-transition metals and sp-elements was presented. In addition, studies of magnetic properties i.e. Invar anomalies $RECo_2$ compounds and interlayer exchange coupling depending on the size of the band gap were presented.

The review continued on Tuesday morning with the co-ordinator's report concerning the Network and the Mid-term report of the Research and Training Network (*http://psi-k.dl.ac.uk/magnetoelectronics/report_2002.html*). W. Temmerman discussed some key points of the report and pointed out that some researchers of the Network were promoted to higher positions, e.g. Stefan Blügel became Director of the Institut für Festkörperforschung (IFF) Institute for Theoretical Physics I in Jülich (Germany). The presentation of the co-ordinator was followed by the meeting between the young researchers and the commission representative.

However, it is known that the present Network ends in 2004 and the EU will not continue with these type of Training Networks. In how far scientific projects will be supported by the EU was presented in the 6th framework talk by R. Monk, the representative from the EU. First of all, he mentioned the general trend that science with direct applications will be preferred in the priority areas, whereas basic research will be less supported. Furthermore, there will be more financing for PhD-students, but less for post-docs. A detailed (provisional) description of the new framework can be found on *http//:www.cordis.lu*.
After the 6th framework talk the Network management meeting started. In the late evening the members of the nodes decided to apply for a new Training Network investigating new materials and novel phenomena in spin-tronics.

Symposium on magnetic semiconductors and half-metallic systems

Half-metals and magnetic semiconductors (SC) have become of interest, because they combine the functionality of semiconductors with the magnetic properties of metals. Therefore, they are candidates for future tunable spin-devices. Three review talks gave an insight on the new developments in this field. Several types of magnetic semiconductors and diluted magnetic SC have been tested in the past, however, in many cases the Curie temperature is too low for practical purposes. Recently, it has been shown that Mn-based diluted magnetic semiconductors are promising systems for spin-tronics, because the T_{C} increases to a reasonable size. A different class of half-metals – GaN or AlN doped with $4f$-rare-earth elements – which should have also a very high T_{C}, was presented by H. Katayama-Yoshida.
The following eight presentations, which were given by node members, showed that the problems of half-metals and magnetic semiconductors are intensively studied in the Network. First, it was shown by R. Mattana from the French node that the new class of materials exhibits a large TMR effect and that in the case of double junctions MR values of similar size can be observed. Second, huge efforts were focussed investigating the electronic structure and the magnetic properties of half-metallic systems and (diluted) magnetic semiconductors, i.e. mostly GaMnAs systems. Some talks were devoted to the calculation of the Curie temperature and the critical temperature combining *ab initio* theory with statistical physics, i.e. Monte Carlo simulations or the Heisenberg model. In addition, an ansatz for the calculation of the phase stability and ordering phenomena in FM SC was given. This ansatz made use of the linearized concentration wave method. As reviewed above, the symposium focussed on a topic of current interest and therefore, all presentations were followed by intense discussions.

The Network thanks Frédéric Petroff for the smooth and effective organization.

Heike C. Herper

Saturday October 5

15:00 15:40	Spin-filter effects in metallic nanowires and nanocontacts (**Ingrid Mertig**)
15:40 16:20	Theoretical aspects of spin-dependent tunneling. (**Juergen Henk**)
16:20 17:00	Coffee
17:00 17:40	The role of transverse spin accumulation in current induced switching of magnetization (**Peter Levy**)
17:40 18:20	Ferromagnet/Semiconductor interfaces (**Susanne Mirbt**)
19:15 20:15	Dinner
20:30 22:30	Posters 1

Poster Session 1

P01	Ab initio study of electronic and magnetic structure of fcc Fe grown on a Cu(100) substrate (**B.Yu.Yavorsky**)
P02	Atomic contacts: stability, stress, electronic structure and magnetism (**A.L. Klavsyuk**)
P03	Spin motion in electron transmission through ultrathin ferromagnetic films (**Juergen Henk**)
P04	Beyond LDA: GW and SIC implementation in KKR (**Arthur Ernst**)
P05	Quantum-size effects in ultrathin Ag films on V(001): Electronic structure and photoelectron spectroscopy (**Arthur Ernst**)
P06	Electronic structure and tunnel magnetoresistance of Fe/MgO/Fe (**M. Bouhassoune**)
P07	In-plane uniaxial anisotropy at the Fe/ZnSe(001) interface (**Lars Nordström**)
P08	An embedded Green-function approach to ballistic electron transport through an interface (**D. Wortmann**)
P09	Ballistic Spin Injection from Fe into ZnSe and GaAs (**O. Wunnicke**)
P10	Ab initio investigations of Fe/W(110): Magnetic Structure of Domain-Walls (**M. Heide**)
P11	Surface core level shift used as a tool to identify PdMn systems on Pd(100) (**W. Olovsson**)
P12	Multiple-scattering theoretical approach to scanning tunneling spectroscopy (**P. Karas**)
P13	Half-ferromagnetism and Slater-Pauling behavior in the Heusler alloys (**I. Galanakis**)
P14	Electronic and magnetic properties of ferromagnet/semiconductor interfaces (**M. Kosuth**)
P15	Relativistic effects in the transport properties of FM/SC/FM trilayer systems (**V. Popescu**)
P16	Probing magnetic susceptibilities using the field-induced magnetic circular dichroism (**S. Mankovsky**)

P17	Disorder-induced magnetism in $TiFe_xCo_{1-x}$ (**D. Benea)**
P18	LMTO Green Function approach for the ab initio calculation of the optical and magnetooptical properties of solids (**S. Chadov)**
P19	Electron-electron interaction viewed by one-photon two-electron excitations (**J. Berakdar)**
P20	Magnetization of the unsegregated and segregayed (100) surface of MoV binary alloy (**L.V. Pourovskii)**
P21	First-principle study of the magnetoresistance effects in magnetic nanocontacts (**A. Bagrets)**
P22	Phase separation at interfaces in $La_{2/3}Ca_{1/3}MnO_3$ (**M. Bibes)**
P23	Magnetic nanostructures on metal surfaces (**V.S. Stepanyuk)**
P24	The influence of hydrogen adsorption on magnetic properties of Ni/Cu(100) surface (**F. Maca)**
P25	Giant Magnetoresistance in carbon nanotubes (**S.P. Athanasopoulos)**
P26	Relativistic calculation of spin-wave spectra in thin magnetic films (**L. Udvardi)**
P27	Exchange interactions in magnetically frustrated systems (**I.A. Abrikosov)**

Sunday October 6

9:00 9:40	Spin-polarized diffusive transport in ferromagnetic metal/semiconductor heterostructures (**Albert Fert)**
9:40 10:20	Proximity Effects Between Superconductors and Ferromagnets (**Balazs Györffy)**
10:20 11:00	Coffee
11:00 11:40	First-principles theory of semiclassical spin and charge transport (**Paul J. Kelly)**
11:40 12:20	Ab initio characterization of the giant magnetoresistance in realistic spin valves (**Laszlo Szunyogh)**
12:30 13:30	Lunch
14:00 19:00	Social Event
19:00 20:15	Dinner
20:30 22:30	Posters 2

Monday October 7

9:00 9:40	Exchange interactions in bulk and layered itinerant magnets (**Ilja Turek)**
9:40 10:20	Half metalic transition metal oxides (**Dzidka Szotek)**
10:30 11:00	Coffee
11:00 11:40	Fundamental tunneling studies using the half-metallic manganite $La_{0.7}Sr_{0.3}MnO_3$ (**Martin Bowen)**
11:40 12:20	Magnetic and transport properties of ferromagnet/semiconductor/ ferromagnet systems (**H. Ebert)**
12:30 13:30	Lunch

14:00 14:30	Study of half-metallicity in LSMO junctions (**G. Banach)**
14:30 15:00	Andreev Bound States and Spontaneous Currents in Ferromagnet - Superconductor Heterostructures (**M. Krawiec)**
15:00 15:30	CPP-transport calculations in Co/Cu (001) and (111) trilayers. (**O. Bengone)**
15:30 16:00	Spin-injection through an Fe/InAs Interfaces (**M. Zwierzycki)**
16:00 16:30	Coffee
16:30 17:00	Perpendicular electric transport in Fe/Si/Fe trilayers: influence of alloying and interdiffusion (**H. Herper)**
17:00 17:30	Towards New Half-Metallic Systems: Zinc-Blende Compounds of Transition Elements with N, P, As, Sb, S, Se and Te (**P. Mavropoulos)**
17:30 18:00	(**P. Vlaic)**
18:00 18:30	Quantitative theory of the Invar anomaly in RECo2 and magnetization processes in Y(Co1-xAlx)2 compounds (**S. Khmelevskyi)**
18:30 18:40	Multiple-scattering theoretical approach to scanning tunneling spectroscopy (**P. Karas)**
18:40 18:50	Bandgap dependence of the interlayer exchange coupling (**T. Dziekan)**
19:00 20:30	Conference Dinner
20:30 21:30	6th Framework Talk
21:30 22:30	Open Network Management Meeting

Tuesday October 8

9:00 10:15	Mid-Term Review
10:15 10:45	Coffee
10:45 12:00	Mid-Term Review
12:00 13:00	Lunch
	Symposium on Magnetic Semiconductors and Half-Metallic Systems
15:00 15:40	Control of spin ordering in ferromagnetic semiconductors (**Tomasz Dietl)**
15:40 16:20	Materials Design of New-Class of Diluted Magnetic Semiconductors by ab initio Electronic Structure Calculation: 4f Rare Earth Metal Doping and 3d Transition Metal Doping (**Hiroshi Katayama-Yoshida)**
16:20 17:00	Coffee
17:00 17:40	On the electronic state of Mn impurities in GaAs (**Thomas Schulthess)**
17:40 18:05	Tunnel magnetoresistance of epitaxial double barrier tunnel junctions based on the ferromagnetic semiconductor GaMnAs (**Richard Mattana)**
18:05 18:30	Electronic and magnetic structure of Cr and Mn doped GaAs (**Olle Eriksson)**
18:30 18:55	Exchange interactions and Curie temperature in (GaMn)As (**L. Sandratskii)**
19:15 20:15	Dinner

9:00 9:25	Ab initio study of group IV and III-V magnetic semiconductors (**J. Kudrnovsky)**
9:25 9:50	Phase stability and ordering in (Ga,Mn)As alloys (**V. Drchal)**
9:50 10:15	Critical temperatures of diluted magnetic semiconductors. (**L.Bergqvist)**
10:15 11:10	Coffee
11:10 11:35	Magnetism in diluted magnetic semiconductors (**B.Sanyal)**
11:35 12:00	Electronic structure and Curie temperatures of diluted magnetic semiconductors (**K. Sato)**
12:00 13:00	Lunch + Closure of Annual Meeting

LECTURES

Spin-filter effects in metallic nanowires and nanocontacts

N.Papanikolaou[a], A.Bagrets[b], J.Opitz[a], P.Zahn[c] and I.Mertig[a]

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[b] *Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany*

[c] *Uppsala Universitet, Fysika Institutionen, SE-75121 Uppsala, Sweden*

We present ab-initio calculations of electronic transport in metallic nanowires and nanocontacts. We consider translationally invariant wires with a diameter of few atoms. The nanocontacts are modeled by short chains of atoms embedded between semi-infinite leads. We used a first-principle screened Korringa-Kohn-Rostoker Green's function method to calculate the electronic structure of the nanowires and nanocontacts. The electronic transport properties were obtained using the Landauer formalism. We have investigated the effect of transition metal impurities on the conductance of the nanowires and nanocontacts. We will demonstrate that single impurities can easily block the conducting channels in nanowires and reduce the conductance. Impurity pairs however cause quantum interference effects and give rise to a complicated energy dependence of the conductance. In nanocontacts we will show how the spin is transmitted through atomic chains and how nanocontacts can act as spinelectronic devices.

Theoretical aspects of spin-dependent tunneling

J. Henk and P. Bruno

Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany

The idea to exploit the electron spin in electronic circuits (spintronic) has lead to a vast amount of both experimental and theoretical work. However, even simple systems—like tunnel junctions which consist of two ferromagnetic electrodes separated by a nonmagnetic spacer—are challenging theory and provide new insights. In this topical review, I shall discuss some theoretical aspects of spin-dependent tunneling.

The first part of the talk is concerned with planar tunnel junctions. Regarded as a scattering process, tunneling can naturally be formulated within multiple-scattering theory (e. g., layer-KKR). Starting from *ab-initio* calculations (DFT, LSDA), the tunneling conductances are obtained from Landauer-Büttiker theory. Besides technical details — like efficient Brillouin zone integration — I shall discuss 'hot spots' in the tunneling transmission of Ni/Vacuum/Ni and the importance of the interface structure for Fe/MgO/Fe. The dependence of the tunnelmagnetoresistance on the bias voltage is addressed for Co/Vacuum/Co.

The second part focuses on scanning tunneling spectroscopy. Formulating the tunneling process within scattering theory provides a straight-forward implementation in multiple-scattering theory which goes beyond the popular Tersoff-Hamann approach. Model calculations reveal the power of this ansatz.

A self-consistent treatment of non-equilibrium spin torques in magnetic multilayers

Peter M. Levy

New York University, USA

The concept of using a spin polarized current to switch the orientation of a magnetic layer was developed by Slonczewski and Berger, and has been followed up by others. Recently, we have proposed a way to understand this spin transfer torque by adopting the model we used to understand magnetoresistance for currents perpendicular to the plane of the layer (CPP), Namely, two phenomena, CPP magnetoresistance (MR) and spin torque, originate from the spin accumulation. The former is primarily associated with the longitudinal spin accumulation and the latter is governed by a transverse effect. The distinguishing feature between previous treatments and the one we recently outlined lies in our focus on the spin transport for the entire CPP structure rather than for the interface region alone, i.e., we consider the spin torque due to the bulk of the magnetic layers and the diffuse scattering at interfaces.

Among the points I plan to higlight in my presentation are that the angular momentum transferred to a thin layer, that is to be switched, far exceeds the transverse component (to the orientation of the magnetization of the thin layer) of the bare portion of the incoming spin polarized current, i.e., that part proportional to the electric field. This is a direct consequence of the spin accumulation coming from the two primary layers, the thick magnetic and nonmagnetic back layers, that produce this buildup. The role of this accumulation in the spin current is a consequence of considering the transport in the multilayer as a diffusive process, and is in keeping with previous treatments of transport in magnetic multilayers. Among other things the parameters entering our theory are determined from CPP transport measurements, except for the exchange interaction between the itinerant electrons and the magnetic background. I will show why this exchange constant is smaller than what can be inferred from LSDA band structure calculations.

Ferromagnet/Semiconductor interfaces

Susanne Mirbt

Condensed Matter theory Group, Uppsala University, Box 530, S-75121 Uppsala, Sweden

We have studied the structural and magnetic properties of Fe on GaAs(100) and ZnSe(100). Calculations involving full geometry optimizations have been carried out for a broad range of thickness of Fe layers (0.5-10 ML) on top of both a GaAs and ZnSe substrate. Both cation and anion terminated interfaces have been explored. Total energy calculations show that the anion segregates at the surface in agreement with experiment.

Spin polarized transport in ferromagnetic metal/semiconductor heterostructures

A. Fert and H. Jaffrès

Unitè Mixte de Physique CNRS-Thalés, Domaine de Corbeville, 91404 Orsay, France, and Universitè Paris-Sud, 91405 Orsay, France.

Tunnel barriers or Schottky contacts at the interface between a ferromagnetic metal and a semiconductor can present interesting spin filtering properties, as this is shown in several communications at this meeting. However having a spin dependent transmission through the interface is not the only condition and, even with a spin dependent tunnel or Shottky junction, the injected current can be non-polarized. This comes from the unbalance between the spin accumulation and relaxation effects in the two materials. This unbalance problem led Schmidt et al [1], a few years ago, to conclude that a spin polarized current cannot be injected from a metal into a semiconductor. In our presentation at Oléron, we will show how one can get round the fundamental difficulty raised by Schmidt et al, and how an efficient spin injection can be achieved. We also discuss the problem of spin transmission and spin detection in several types of ferromagnetic metal/semiconductor heterostructures. By adapting the spin accumulation model of the perpendicular transport in metallic magnetic multilayers to the situation of ferromagnetic metal (F)/semiconductor (SC) heterostructures [2], we show that the problem of spin injection between F and SC can be solved by introducing a well-adapted spin dependent interface resistance (tunnel junction preferably) at the F/SC interfaces. In the little more complex situation of a F/SC/F structure, a significant value of the magnetoresistance (signature of spin injection + electrical spin detection) can be obtained if the junction resistance is chosen between two threshold values depending on the resistivity, spin diffusion length and thickness of SC. We illustrate the results of our model with numerical calculations for Co/GaAs/Co structures. Our results on F/SC/N structures are at odds with recent theoretical results of Rashba [3] and we explain the origin of the discrepancy. Finally we will present extensions of our approach to other types of geometry (injection into a 2DEG, double tunnel junctions, etc). We will also discuss interesting effects expected for high current densities.

[1] G. Schmidt et al., *Phys. Rev. B* **62**, 4790 (2000)

[2] A. Fert, H. Jaffrès, *Phys. Rev. B* **64**, 184420 (2001)

[3] E. Rashba, *Phys. Rev. B* **62**, 16267 (2000)

Proximity Effects Between Superconductors and Ferromagnets

Balazs L. Györffy
University of Bristol, UK

As has been discovered in the 1960-ies a superconductor in contact with a normal metal can induce pairing correlations in the latter. Although this, surprising, Proximity Effect is by now well understood a version of it which occurs when the normal metal is ferromagnetic is attracting current interest. I shall review the recent advances in our understanding of the Proximity Effect in such hetero structures and argue that they are of both scientific and technological interest. In particular I will emphasis the unique role they can play in the study of interaction between magnetism and superconductivity and comment on their significance in the context of spin-dependent transport.

First-principles theory of semiclassical spin and charge transport

Paul J. Kelly
Faculty of Applied Physics and MESA+ Research Institute,
University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Spin and charge transport in the semiclassical regime is governed by the scattering matrices of interfaces which connect the distribution functions in the bulk materials on either side. We review the results of first-principles calculations of the scattering matrix as applied to various physical properties like spin-dependent interface resistances, Andreev scattering, spin current-induced magnetization torque, angular magnetoresistance, Gilbert damping of magnetization dynamics and spin-injection into semiconductors. We emphasize the importance of interface disorder and the phase of the elements of the scattering matrix and, where available, compare theoretical results with experiments.

Ab initio characterization of the giant magnetoresistance in realistic spin valves

P. Weinberger
Technical University of Vienna, Austria

L. Szunyogh
Budapest University of Technology, Hungary

The electric transport properties of a rather complicated spin valve system containing NiFe permalloy, CoFe hard magnets and two types of spacers (Cu,Ru) are investigated theoretically in terms of the of the Screened Korringa-Kohn-Rostoker method and the Kubo-Greenwood equation. It is found that the regimes of antiferromagnetic coupling are mostly determined by the thickness of the Cu spacer: the nodes of oscillation of the interlayer exchange coupling (IEC) with respect to the Cu spacer thickness are shifted only marginally by the presence of a very thin Ru spacer. The oscillations of the IEC and the giant magnetoresistance

(GMR) are investigated with respect to the thickness of the hard magnet parts of the system (CoFe). The minima viewed with respect to the thickness of the Cu spacer and also the actual values of the GMR are in reasonable agreement with experiment.

Exchange interactions in bulk and layered itinerant magnets

I. Turek

Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno

J. Kudrnovský, V. Drchal

Institute of Physics, Acad. Sci. Czech Rep., Prague

P. Bruno

MPI für Mikrostrukturphysik, Halle, Germany

S. Blügel

Institut für Festkörperforschung, FZ Jülich, Germany

The talk reviews a two-step procedure to determine thermodynamic properties of itinerant magnets from first principles. In the first step, the selfconsistent electronic structure of a system is calculated using the tight-binding linear muffin-tin orbital method combined with Green function techniques, which is appropriate for description of substitutional randomness of disordered bulk alloys and for two-dimensional translational periodicity of layered systems like surfaces and thin films. In the second step, the parameters of the effective classical Heisenberg Hamiltonian are determined using the magnetic force theorem and they are employed in subsequent evaluation of magnon spectra, the spin-wave stiffness constants and critical temperatures. Examples of application include: (i) ferromagnetic $3d$ metals Fe, Co, and Ni, (ii) disordered binary transition-metal alloys, (iii) ultrathin magnetic films of Fe and Co on a Cu(001) substrate, (iv) diluted magnetic semiconductors (Ga,Mn)As, and (v) $4f$ electron systems like hcp Gd and bcc Eu. The developed theory will be presented together with selected aspects of the numerical implementation and with a comparison to existing experimental data.

Half-metallic transition metal oxides

Z. Szotek

Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

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.

Fundamental tunneling studies using the half-metallic manganite $La_{0.7}Sr_{0.3}MnO_3$

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To better understand certain fundamental aspects of tunneling, we have integrated the half-metallic manganite $La_{0.7}Sr_{0.3}MnO_3$ (001) (LSMO), grown in an epitaxial bilayer with an insulating barrier of $SrTiO_3$(001) (STO), into magnetic tunnel junctions. LSMO/STO/LSMO junctions yield up to 1800% magnetoresistance for a LSMO spin polarization in excess of 95% [1], and reveal band structure features in the bias dependence of magnetoresistance in agreement with inverse photoemission experiments [2] performed on LSMO/STO(001) and STO(2ML)/LSMO/STO(001). Conductance studies at high magnetic fields point to a departure in tunneling behavior from interfacial 2D to 3D as the result of using junction electrodes with a more delocalized double exchange conduction mechanism rather than the more conventional metallic behavior of transition ferromagnets. Finally, to understand the influence of the epitaxial barrier on tunneling, we will present preliminary transport results on LSMO-based junctions which integrate an epitaxial TiO_2 barrier [4].

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Electronic and magnetic and transport properties of ferromagnet-semiconductor heterostructure systems

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The electronic and magnetic and transport properties of ferromagnet/semiconductor (FM/SC) heterostructure systems have been studied by means of various band structure methods (LMTO, KKR-CPA, TB-KKR). As a structural model for our calculations periodic multilayer systems as well as half-infinite tri-layer systems have been assumed, taking for the ferromagnet Fe and for the semiconductor GaAs or Ge. Together with the profile of the spin and orbital magnetisation the magneto-crystalline anisotropy has been investigated in detail to check the relationship between the electronic magneto-crystalline anisotropy energy and the anisotropy of the orbital moment as proposed by van der Laan. Making use of the Coherent Potential Approximation

(CPA), the influence of interdiffusion at the Fe/GaAs interface within the multilayer system has been studied. On the basis of the electronic structure calculations, the magnetic circular X-ray dichroism (MCXD) has been calculated for the L_3-edges absorption spectra of Fe, Ga and As in the near-edge regime (XANES). The transport properties of FM/SC heterostructure systems were studied by making use of a relaxation time approach. The results were combined with data for the exchange coupling to give the conductivity as a function of an external magnetic field. In addition to these model studies first principle calculations of the conductance of FM/SC tri-layer systems have been made using the TB-KKR method in combination with the Landauer Büttiker formalism. Attention has been paid in particular to the influence of the spin-orbit coupling. It turned out the TMR ratio can be reduced in a rather appreciable way by the spin-orbit coupling with the conductance of the anti-ferromagnetic configuration more influenced than the ferromagnetic one.

Study of half-metallicity in LSMO junctions.

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We perform one-electron calculations for $La_{1-x}Sr_xMnO_3$ (LSMO) and $SrTiO_3$ (STO), and for the surfaces of these materials, and also the interface of LSMO/STO. TB-LMTO-LSDA and SIC-LSDA LMTO-ASA methods were used. The calculations for nonstochiometric perovskites were based on a stochiometric supercell model ($[La_2SrMnO3]_n$, where n=1, 2, 3) and a rigid band model. We confirmed earlier results of Picket and Singh [1] for LSMO, a strongly polarised electronic structure, nearly half-metallic was obtained. From SIC-LMTO calculations we found a half-metallic state for LSMO for manganese configuration Mn^{+3}, where the localised electrons are the $3t_{2g}$ and one e_g. The supercell method was used to model LSMO and STO surfaces. A first calculation for the junction LSMO/STO/LSMO was accomplished for interface MnO/SrO.

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Andreev Bound States and Spontaneous Currents in Ferromagnet - Superconductor Heterostructures

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We discuss the ground state properties of an 'insulator - ferromagnet - superconductor' trilayer on the basis of a Hubbard Model featuring exchange splitting in the ferromagnet and electron - electron attraction in the superconductor. We have solved the spin - polarized Hartree - Fock - Gorkov equations together with the Maxwell's equation (Ampere's law) fully self-consistently. We have found that due to proximity effect the $FFLO$ - like state [1,2] is realized in such a heterostructure. It manifests itself in oscillatory behavior of the pairing amplitude in the FM and a spontaneously generated spin - polarized current (and magnetic field) in the ground state of the system [3]. We shall discuss the presence of the Andreev bound states, the position of which can be tuned by exchange splitting, and its relation to the current and the pairing

amplitude. Finally we will also mention the spin polarization of the current, which is very sensitive to the band filling.

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CPP-transport calculations in Co/Cu (001) and (111) trilayers.

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A Kubo-Landauer conductance calculation method in the perpendicular geometry, based on transmission matrix formulation has been adapted and implemented in a TB-LMTO-ASA code for general crystallographic orientations of layers. Disorder effects, such as interdiffusion at the interfaces and impurities in different layers, are treated by means of a two dimensions lateral disordered supercell with random distribution of atoms. The present implementation has been applied to Co/Cu trilayers in the fcc (001) and (111) crystallographic orientations. In case of Cr impurity in CoCr/Cu/Co (111) trilayers, an inverse GMR effect is found depending on the magnetic layer thickness, in accordance with experiment.

Spin-injection through an Fe/InAs Interfaces

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The basic obstacle to spin-injection from a metallic ferromagnet into a semiconductor is the large difference in their conductivities; the resistivity of a semiconductor such as InAs is much larger than either the majority- or minority-spin resistivity of Fe. However, the spin-dependent interface resistance if sufficiently large could generate a spin-dependent potential drop at the interface. Here, we evaluate this term for an Fe/InAs interface from first principles. The formalism based on the tight-binding linear-muffin-tin orbital surface Green's function method allows us to treat large lateral superlattices so that we can study the influence of disorder on the conductance. We find that due to the symmetry mismatch in the minority-spin channel the specular interface acts as an efficient spin filter with the polarisation of transmitted current

close to 100%. The resistance of a diffusive interface is comparable to the resistance of an InAs slab several hundreds nanometers thick but the symmetry breaking due to the disorder can substantially reduce the spin-asymmetry. We conclude that the spin injection for this system is possible only if the interface disorder is not too large.

Perpendicular electric transport in Fe/Si/Fe trilayers: influence of alloying and interdiffusion

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We have investigated the electric transport properties of Fe/Si/Fe trilayers in current perpendicular to the plane (CPP) geometry and the interlayer exchange coupling (IEC) depending on the Si layer thickness. Additional effort has been done by examing the influence of interdiffusion, alloy formation at the interfaces, and homogeneous FeSi spacers on the GMR and IEC, because Fe and Si tend to form CsCl-like alloys. It is known from a number of experiments that Fe/Si trilayers or superlattices show a small GMR effect varying between 0.1 and 2.2 %. We have been able to demonstrate that this small values for the GMR are related to the existence of interdiffusion at the Fe-Si interfaces. A 5 % interdiffusion is already sufficient to decrease the GMR by 50 % and a interdiffusion concentration of 50 % leads to small values of the GMR, which are of the same size as the experimental data. Furthermore, it has been shown that these interdiffusion effects also stabilize the AF interlayer exchange coupling.

The electronic calculations have been performed within the fully relativistic spin-polarized version of the Screened KKR method. The transport properties e.g. the resistances have been determined by using the fully relativistic spin-polarized Kubo-Greenwood equation.

Towards New Half-Metallic Systems: Zinc-Blende Compounds of Transition Elements with N, P, As, Sb , S, Se, and Te

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We have studied zinc-blende compounds of the transition metal elements V, Cr, Mn with the sp elements N, P, As, Sb, S, Se, Te. In the ferromagnetic configuration they all show a tendency towards half-metallic behavior, *i.e.* a band gap in the minority density of states resulting in 100% spin polarization at E_F. This can be traced back to the bonding-antibonding splitting due to hybridization between the transition element d (t_{2g}) states and the sp element p states, conspiring with the large exchange splitting which pushes up the minority d states. The total moment M per unit cell, if the system is half-metallic, is integer and given by the $M = Z - 8$, where Z is the number of valence electrons per unit cell. Also, the sp atoms are found to

have an antiparallel local moment with respect to the $3d$ atoms. The electronic and magnetic properties of all these compounds show strong similarities to the corresponding dilute magnetic semiconductors.

We discuss the trends with varying lattice constant, in view of the possibility to grow these materials epitaxially on various semiconductors. Compression eventually kills half-metallicity, since E_F finally wanders above the minority gap. However, for compounds involving lighter sp elements half-metallicity is encouragingly more robust; this can be explained in terms of the stronger local moment close to the $3d$ atom for lighter sp elements, resulting in a larger exchange splitting and gap.

Finally, we have examined the behavior of the transition element terminated (001) surfaces. In most cases half metallicity is maintained, and the magnetic moment increases because of the missing neighbours where charge would be transfered. Exceptions are the cases where the surface magnetic moment should exceed 5 μ_B, for which half metallicity is lost.

Quantitative theory of the Invar anomaly in RECo2 and magnetization processes in $Y(Co_{1-x}Al_x)_2$ compounds

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We show that the large negative magnetic contribution to the thermal expansion in $DyCo_2$ and $HoCo_2$ can be understood within the s-d (d-f) model. The Invar anomaly in these compounds appears to be a consequence of the metamagnetic properties of the Co sublattice, treated by ab-initio calculations, and the rare-earth local moments coupled to it. It is found, that all finite temperature dynamics of the Invar effect is exclusively governed by the magnetic excitations of the rare-earth moments. Based on TB-LMTO CPA calculations we disscuss a problem, which has been debated in the literature for the recent years, namely the possibility of a metamagnetic transition in $Y(Co_{1-x}Al_x)_2$ with $x > 0.12$. Using the Stoner model, but based on actually calculated DOS of $Y(Co_{1-x}Al_x)_2$, we study the high-field magnetisation process in these compounds. The results of our investigation suggest that independent of the choice of the Stoner parameter no metamagnetic phase transition occurs above the critical concentration. It is shown that this conclusion is independent on the actual value of the exchange interaction in the system due to peculiar changes in the shape of the density of states with alloying.

Multiple-scattering theoretical approach to scanning tunneling spectroscopy

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The qualitative and quantitative theoretical description of scanning tunneling spectroscopy (STS) is usually based on the popular Tersoff-Hamann model. By simply relating the tunneling current to the spectral density of the sample, however, relevant properties of the tunneling through the tip-sample system are neglected.

Viewing electronic tunneling as a scattering process, we present a formulation of STS in terms of multiple-scattering theory which takes into account the tip-sample interaction. Further, electronic properties of the constituent systems can be obtained by ab-initio calculations. Besides a presentation of the general formalism and its implementation in a spin-polarised relativistic layer-KKR scheme, we sketch results for prototypical systems, with a focus on features of the scattering-theoretical approach.

Bandgap dependence of the interlayer exchange coupling

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LDA method is widely used in solid state physics. But among other things it reproduces the bandgap of semiconductors like GaAs not accurate enough. LDA+U is one approach to overcome this problem. After a short motivation for the choise of the fitting parameter U in GaAs, LDA+U is applied on the Fe—GaAs—Fe multilayer system. We find an increased interlayer exchange coupling with increased bandgap.

Symposium on Magnetic Semiconductors and Half-Metallic Systems

Control of spin ordering in ferromagnetic semiconductors

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Recent advances [1] in the field of carrier-controlled ferromagnetism in tetrahedrally coordinated diluted magnetic semiconductors and their nanostructures will be reviewed with a focus on the phenomena important for prospective spintronic devices. Experimental results for III-V materials, where the Mn atoms introduce both spins and holes [1,2], will be compared to the case of II-VI compounds, in which the Curie temperatures TC above 1 K have been observed for the uniformly [3] and modulation-doped p-type structures [4] but not in the case of n-type films. The experiments demonstrating the tunability of TC by light [4] and electric field [4,5] will be presented. The tailoring of domain structures and magnetic anisotropy by strain engineering [2,6] and confinement [4] will be discussed emphasizing the role of the spin-orbit coupling in the valence band. The question of designing modulated magnetic structures in low dimensional semiconductor systems will be addressed. Recent progress in search for semiconductors with TC above room temperature and hopes associated with materials containing magnetic ions other than Mn will be presented [1,2].

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Materials Design of New-Class of Diluted Magnetic Semiconductors by ab initio Electronic Structure Calculation: 4f Rare Earth Metal Doping and 3d Transition Metal Doping

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I will discuss the materials design of new-class of diluted magnetic semiconductors based upon ab initio electronic structure calculations. Rare-earth ions doped in semiconductors have been very interesting and attractive for applications to fiber communications as well as medical sensing and surgery. We have succeeded in predicting a new-class of half-metallic ferromagnetic semiconductors doped by rare-earth ions to various wide-band gap III-V semiconductors such as AlN and GaN, which result in drastic enhancement of ferromagnetism due to intra-4f shell of rare-earth ions in the impurity bands. Based upon the total energy calculation between the ferromagnetic states and spin glass states, we have designed the following new-class of ferromagnetic semiconductors. (i) Ce-, Pr-, Nd-, Pm-, Sm-, Eu, Ho- Er-doped GaN and AlN show the half-metallic ferromagnetism. Ce- (5%) doped AlN and GaN show T_c up to 500K without any doping treatment. Gd-doped GaN and AlN is spin glass state, however, electron doping stabilized half-metallic ferromagnetism. (ii) Ce-doped silicon shows the very high Curie temperature (T_c) up to 6000K.

We also designed the ferromagnetic semiconductors in 3d transition atom doped IV semiconductors such as diamond (C), silicon (Si) and germanium (Ge). Based upon the total energy calculation between the ferromagnetic states and spin glass states, we have designed the following new class of ferromagnetic IV-th semiconductors. (iii) 3d transition atom doped diamond never show the ferromagnetism because of the strong delocalization of valence and impurity band caused by the too strong p-d hybridization (small lattice constant). (iv) Substitutional Mn-, Fe-, and Co-doped Ge and Si show the ferromagnetism, however, Co-doped Ge is low-spin ground state. Fe-doped Ge and Si is the most stable ferromagnet with high-T_c. (v) Interstitial 3d

transition metal doped Ge and Si never show the ferromagnetism because of the delocalization of t2 and e-states due to the strong p-d hybridization.

I will discuss the mechanism of high-T_c in the above new systems based upon the competition between the p-d exchange interaction and double exchange interaction. We concluded that the high-T_c is realized based upon the double exchange mechanism, in which stabilization energy caused by the partially occupied itinerant 4f and 3d impurity band dominate the ferromagnetism with high-T_c. Low-T_c may be caused by p-d (p-f) exchange interaction.

On the electronic state of Mn impurities in GaAs

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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 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 only four Mn d states are filled with an acceptor states that is localized to the Mn impurity and the first As neighbor shell. 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 a GaAs host 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. For GaMn-As we find that the self interaction corrections strongly affect the electronic state of Mn. The majority d orbitals are no longer hybridized and are all occupied leaving Mn nominally with S=5/2. The nature of the acceptor states changes as well, in that they have mainly p character and are no longer localized to the Mn site and its nearest neighbors.

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Tunnel magnetoresistance of epitaxial double barrier tunnel junctions based on the ferromagnetic semiconductor GaMnAs

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For spin injection into semiconductors, magnetic semiconductors are an alternative to ferromagnetic metals, with the advantage that the difficulties resulting from the conductivity mismatch between metals and semiconductors can be avoided. On the other hand, magnetic tunnel junctions with magnetic semiconductor electrodes can be used to test spin injection since the existence of tunnel magnetoresistance (TMR) is a signature of the transmission of spin-polarized carriers between the electrodes [1]. We have fabricated single and double barrier magnetic tunnel junctions with GaMnAs electrodes by a low temperature molecular beam epitaxy procedure. The two magnetic electrodes ($Ga_{(1-x)}Mn_xAs$) are separated by a thin AlAs (17) tunnel barrier (single barrier MTJ) or by a AlAs(17)/GaAs(50)/AlAs(17) trilayer (double barrier MTJ). Antiparallel arrangement of the ferromagnetic electrodes at low field is obtained by varying the thickness and Mn concentration in the GaMnAs layers in order to obtain different coercive fields. GaAs layers have been inserted between the electrodes and tunnel barrier in order to avoid the diffusion of Mn into the tunnel barrier. We observe large TMR effects, 38% at low field and 650% at 5 T in the single junction after progressive saturation of the electrode magnetisation. The existence of similar large MR ratios in the double junction is a new and interesting effect, never observed in metallic double junctions when the intermediate electrode is nonmagnetic. This can be ascribed to the non- relaxed spin splitting of the chemical potential predicted for an intermediate semiconductor electrode [2].

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Electronic and magnetic structure of Cr and Mn doped GaAs

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The electronic strycture and magnetic properties of Mn and Cr doped GaAs are reviewed. The effect of lattice relaxation on the magnetic properties are described [1] as well as the effect of lattice impurities[2]. Theoretical values of magnetic moments and critical temperatures are compared to experimental data and avenues for improving the magnetic properties are discussed. In addition phase stability of the Mn-GaAs and Cr-GaAs systems are discussed both for the ideal, defect free case, as well as for the case with As antisite defects[3].

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Exchange interactions and Curie temperature in (GaMn)As

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We use supercell and frozen-magnon approaches to study the dependence of the magnetic interactions in (Ga,Mn)As on the Mn concentration. We report the parameters of the exchange interaction between Mn spins and the approximations. In agreement with experiment we obtain a nonmonotonous dependence of the Curie temperature on the Mn concentration. We estimate the dependence of the Curie temperature on the concentration of the carries in the system and show that the decrease of the number of holes in the valence band leads to fast decrease of the Curie temperature. We show that the hole states of the valence band are more efficient in mediating the exchange interaction between Mn spins than the electron states of the conduction band.

Ab initio study of group IV and III-V magnetic semiconductors

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The electronic structure of diluted GeMn and (Ga,Mn)As magnetic semiconductors is studied from first principles with a particular emphasis on the effect of various kinds of defects. We map total energies associated with rotations of the Mn-magnetic moments onto an effective Heisenberg Hamiltonian which is then treated in the mean-field approximation in order to find the Curie temperature. The presence of donors like e.g. As-antisites in GaMnAs strongly reduces the Curie temperature. The Heisenberg exchange interactions are reduced with increasing concentrations of both Mn and As in GaMnAs and with increasing concentrations of Mn in GeMn. Calculations indicate an increase of the donor concentration with the increase of the Mn-content in GaMnAs. Finally, we have also investigated the effect of electron correlations included in the framework of the LDA+U method on the properties of GaMnAs alloys.

Phase stability and ordering in (Ga,Mn)As alloys

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The phase stability and the possible ordering in ferromagnetic semiconducting alloys is studied from first principles. We determine first the total energies of disordered alloys as a function of their chemical composition. In a next step, by using the generalized perturbation method,

we evaluate effective interatomic interactions between impurities by taking into account also the electrostatic interactions. Finally, by employing the methods of statistical physics, namely, by using the linearized version of the concentration wave method we determine the ordering temperature and the k-vector of the transition from the disordered to the ordered state. For temperatures above the ordering temperature we finally calculate the Warren-Cowley short-range order parameters which yield information about the spatial correlation of impurities. As an illustration, we present results for (Ga,Mn)As alloys.

Critical temperatures of diluted magnetic semiconductors.

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We have systematically calculated critical temperatures of several diluted magnetic semiconductor systems doped with mangenese using supercell and frozen-magnon approaches. By fitting the spin wave energies, using the force theorem, to a Heisenberg expression for magnetic ordering, we have extracted the exchange interactions between the Mn ions. The critical temperatures have been estimated from Monte Carlo simulations and in the few cases where they could be compared with earlier calculations, we find that our approach usually give values between the critical temperatures estimated from mean field and random phase approximations.

Magnetism in diluted magnetic semiconductors

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Diluted magnetic semiconductors (DMS) are crucial ingradients in magnetoelectronics and semiconductor technology. III-V semiconductors doped with 3d transition metals especially Mn, are the mostly studied materials nowadays. We will present ab-initio electronic structure calculations of transition metal doped semiconductors. Calculations done for various aspects e.g. influence of defects in a Mn doped GaAs system will be shown. Also, to explore the magnetism in a semiconducting host, we will show a comparative study of III-V, II-VI and IV-IV DMSs. Some comments about the exchange interactions in these systems will be made. Lastly, we will present a simple model to understand the magnetism in DMSs.

Electronic structure and Curie temperatures of diluted magnetic semiconductors

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Recent discovery of the carrier induced ferromagnetism in (In, Mn)As and (Ga, Mn)As encourages many experimental and theoretical studies on diluted magnetic semiconductors (DMS), because DMS are candidates for new functional materials whose magnetic properties are controllable by changing the carrier density. In this paper, the electronic structure of several III-V and II-VI DMS is calculated based on density functional theory, and an estimation of their Curie temperature (T_c) is given. The electronic structure is calculated by using the Korringa-Kohn-Rostoker method combined with the coherent potential approximation in order 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. Carrier doping effects are also simulated by this method.

In (Ga, Cr)N, (Ga, Cr)As and (Ga, Mn)N, very large T_c's above room temperature are predicted in realistic concentration ranges. In particular, it is found that the Cr-doped compounds are promising candidates for high-T_c ferromagnets. Room-temperature ferromagnetism is also predicted in (Zn, V)Se, (Zn, Cr)Se, (Zn, V)Te and (Zn, Cr)Te. It is also found that T_c's decrease sharply by electron doping in (Ga, Mn)As and (Ga, Mn)N. In order to discuss the origin of the ferromagnetism, the Curie temperatures of Mn-doped GaN, GaP, GaAs and GaSb are systematically evaluated. Interestingly, they show very different concentration dependences. For low concentrations, the T_c's are approximately proportional to the square root of Mn concentrations in GaN, GaP and GaAs. In particular, in case of GaN, a strong correlation between T_c and the half width of the impurity d-band is observed indicating that the double exchange mechanism dominates. On the other hand, T_c is almost linearly proportional to Mn concentration in (Ga, Mn)Sb. In this case, Mn-3d states have a negligible amplitude at the Fermi level, and the ferromagnetism is stabilized by the p-d exchange interaction. (Ga, Mn)P and (Ga, Mn)As are intermediate cases and it is difficult to say which mechanism dominates.

POSTER SESSION

Ab initio study of electronic and magnetic structure of fcc Fe grown on a Cu(100) substrate.

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Thin films of fcc Fe stabilized by epitaxial growth on a Cu(100) substrate have been a subject of great interest for both experimenatlists and theoreticians. The question of the ground magnetic state of the fcc Fe, however, is still open. In the recent experimental study of Qian et.al [1] a non-collinear magnetic order in this system is discussed.

We have studied the electronic structure of the thin films of fcc Fe on a Cu(100) substrate theoretically by means of the screened KKR method. The system was modeled by a finite slab

of 8 atomic layers of Cu sandwiched by 6 atomic layers of Fe on the both sides. The densities of states and the total energies of the ferromagnetic, the antiferromagnetic, and the non-collinear magnetic structure are presented. The possible magnetic ground state of the system is discussed.

[1] D. Qian, X. F. Jin, J. Barthel, M. Klaua, and J. Kirschner, *Phys.Rev. Lett.* **87**, 227204 (2001)

Atomic contacts: stability, stress, electronic structure and magnetism

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Using KKR Green's function method for low-dimensional systems and density functional theory we construct many body interatomic potentials for atomic contacts. Potentials are formulated in the second-moment tight binding approximation. The parameters of potentials are optimized simultaneusly by including in the fit the results of the first principle calculations of selected cluster-substrate properties, forces acting on adatoms and ab initio bulk properties. We concentrate on the 3d atomic contacts. Atomic scale simulations reveal the interplay between the stability of nanocontacts, stress and electronic structure. We also discuss magnetic nanocontacts and show that that magnetic bridges can exhibit many interesting properties.

Spin motion in electron transmission through ultrathin ferromagnetic films

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The spin-dependent scattering of electrons at interfaces and ultrathin films has a considerable effect on the transport properties of 'spintronic' devices. In this contribution, we report on 'theoretical experiments' which provide direct access to the spin motion of electrons transmitted through 1–6 ML Fe on Pd(001). Spin- and angle-resolved photoelectron spectroscopy from core levels serves as microscopic probe. The spin polarization $P_{\rm in}$ of the incoming photoelectrons (which were excited from a Pd core level) can easily be adjusted by choosing the incidence direction and the polarization of the incident light. Elastic scattering in the Fe films shows up as precession of the spin-polarization vector $\vec{P}$, whereas inelastic effects result in a rotation of $\vec{P}$ towards the magnetization $\vec{M}$. Significant structures in the constant-initial-state photoemission spectra are related to the electronic structures of the Pd substrate and of the Fe film.

Beyond LDA: *GW* and SIC implementation in KKR

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Ab-initio studies of semiconductors and insulators as well as of systems with strongly localized electrons entail great difficulties involved by the treatment of excitation energies and by many-body effects. The most successful first-principles method, the density-functional theory within the local-density approximation (LDA), is designed for ground-state properties and, hence, cannot provide a proper description of the electronic structures of semiconductors and insulators.

If localized electrons are present in the system, the LDA can be essentially improved by the self-interaction correction (SIC). This way, the self-interactions of single-particle charges, which are present in the LDA, cancel out for the localized electrons. However, SIC in conjunction with LDA is still not sufficient for a proper description of excitation energies and band gaps. For an accurate first-principles treatment, one would solve Hedin's set of equations for the full Green's function. Because a complete implementation of this formalism is very difficult, one usually neglects the vertex correction (random-phase approximation), and the self-energy is calculated within the *GW* approximation (GWA). The non-self-consistent GWA was successfully implemented within several first-principles methods, but most of the existing implementations are generally designed for systems with delocalized electrons.

Here, a general *ab-initio* approach for the study of electronic properties of solids is presented. Basing on the Korringa-Kohn-Rostoker (KKR) method, we implemented the SIC for strongly localized electrons and the non-self-consistent GWA for the inclusion of many-body effects. Our approach is illustrated by electronic-structure calculations for semiconductors and transition-metal oxides.

Quantum-size effects in ultrathin Ag films on V(001): Electronic structure and photoelectron spectroscopy

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First-principles calculations are performed to investigate in detail the electronic structure of ultrathin Ag films deposited on V(001). Quantum-well states in the Ag films show the typical dispersion with film thickness, but their spectral densities differ significantly from those of model systems. *Ab-initio* calculations for several systems (bulk, surfaces, interfaces, and thin films) reveal as origins band-structure effects and hybridization between Ag and V states. Quantization effects show up as intensity oscillations in the constant-initial-state mode of photoelectron spectroscopy. Earlier experimental investigations, which reported inconsistencies with typical manifestations of quantization effects, are discussed.

Electronic structure and tunnel magnetoresistance of Fe/MgO/Fe

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Understanding of tunneling magnetoresistance (TMR) is necessary for the important development and fabrication of magnetic tunnel junctions (MTJ) used in non-volatile memories (Magnetic RAM). A prototypical system for such a tunnel junction is Fe/MgO/Fe. It has the advantage that the insulating material is ordered and therefore well characterised. Recent work from an experimental group at the Max-Planck institute in Halle [Phys. Rev. Lett. **87** 076102 (2001)] established that an FeO interface layer is grown between Fe and MgO and that a substantial interface relaxation takes place.

We have started a systematic study on how the electronic structure is affected by (1) interfacial structural relaxation, (2) oxidation of the Fe interface layer, (3) correlation effects in the FeO interface layer, and (4) non-stoichiometry in the FeO interface layer. In conjunction with this we also investigate how these effects influence the tunnelling conductance. Our specific findings so far are: (1) structural relaxation at the interface induces an anti-parallel Fe spin magnetic moment in the layer adjacent to the Fe interface layer, (2) a substantially enhanced Fe spin moment in the interface layer is due to oxidation induced correlation effects, and (3) the spectral functions at the Fermi level with and without oxidation of the Fe interface layer differ quite dramatically.

In-plane uniaxial anisotropy at the Fe/ZnSe(001) interface

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We present a detailed study of the in-plane magnetocrystalline anisotropy (MCA) and its connection to the electronic bonding at an interface between a cubic ferromagnet and a cubic semiconductor, Fe/ZnSe(001). In particular, a uniaxial MCA is found. This is maybe surprising since the calculations are for perfect interfaces, but the effect is traced down to the sp^3-bonding between the semiconductor and the first monolayer of Fe. A uniaxial in-plane MCA is consistent with what is observed in general for bcc Fe/semiconductor interfaces, which jas been a puzzle since its first observation. We will discuss our results in connection with existing models. It is also shown how this uniaxial symmetry is cancelled in a multilayer structures, leading to fourfold anisotropy. The calculations were performed using a full-potential linearized augmented planewave method (FP-APW+lo), which is a computationally more efficient version of the traditionally linearized metod, FLAPW. The spin-orbit induced MCA was studied through the force theorem, as well as through fully relativistic self-consistent calculations. The magnetic anisotropy is presented for several different Fe/ZnSe(001) systems, with three or five monolayers

of Fe grown on a five atoms thick representation of the semiconductor, and with Zn terminated as well as Se terminated semiconductor interfaces.

An embedded Green-function approach to ballistic electron transport through an interface

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We present an efficient method for calculating the conductance of ballistic electrons through magnetic interfaces from first-principles using the embedding approach of Inglesfield [1]. In our method the Landauer-Buttiker formula [2] 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. The embedding formulation was implemented within the framework of the full-potential linearized augmented plane wave (FLAPW) method using the FLEUR code [3]. The actual implementation is discussed in detail. We will present calculations for magnetic multilayer structures used in giant magneto- resistance (GMR) and tunneling magneto-resistance (TMR) devices. In order to check the accuracy, and to allow a comparison with previous calculations we have chosen as an example of a GMR system, the Cu/Co/Cu(100) sandwich structure which is a model system in magneto- electronics and intensively investigated before. As a second application we present the investigation of the spin-resolved electronic tunneling through a Fe/MgO/Fe TMR junction.

[1] J.E. Inglesfield, *J. Phys. C* **14**, 3795 (1981).

[2] M. Buttiker, *Phys. Rev. Lett.* **57**, 1761 (1986).

[3] http://www.flapw.de

Ballistic Spin Injection from Fe into ZnSe and GaAs

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We have investigated the ballistic spin injection from Fe into the semiconductors ZnSe and GaAs by means of an *ab initio* method. The results show a very high spin polarization up to 99% for the [001] growth direction and nearly no spin polarization for the [111] and [110] direction. The origin of the high spin polarization for the [001] direction are the different symmetries of the majority and minority spin wave functions. So we call it a symmetry enforced high spin polarization. This effect is absent for the other investigated directions, i.e., the [111] and [110] direction.

The calculation of the ground state properties is based on the density functional theory within the local density approximation and uses the screened KKR-Green's function method. The conductance is calculated by the Landauer-Büttiker formula in a Green's function description.

We have investigated three different injection processes: (*i*) the injection of hot electrons directly into the conduction band of the semiconductor, (*ii*) the injection of thermal electrons at the Fermi energy without and (*iii*) including a Schottky barrier at the interface.

If a Schottky barrier is included at the interface, new effects from resonant interface states can come in. They can dominate the tunnel current and can even change the sign of the current polarization, e.g., in the Zn terminated Fe/ZnSe(001) interface. Also we have calculated the interface resistance of the Schottky barrier in the (001) orientation as an input value for the analytical models of spin injection through a tunneling barrier proposed independently by Rashba and Fert *et al.* By this we can roughly estimate the required thickness of the Schottky barrier to be 70Å for Fe/ZnSe and 100Å for Fe/GaAs(001).

Ab initio investigations of Fe/W(110): Magnetic Structure of Domain-Walls

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Atomically thin Fe films on the W(110) surface form a two-dimensional ferromagnetic domain structure. From experiments with spin-polarized STM it is known that the magnetization direction in the domains and the width of the walls between two adjacent domains are different for mono- and double-layer Fe coverage. For a mono-layer the wall width is on the atomic scale, while for a double layer the walls are extended over several atomic rows (around 8nm).

The shape of the walls is determined by the competition of the forces caused by spin-stiffness, spin-orbit coupling and magnetic dipolar interactions. In this poster we describe the walls with a simple model and investigate the possibilities and limits of obtaining the required parameters by ab initio calculations. The calculations are performed with the FLAPW-method based on density functional theory.

[e.g. M. Pratzer *et. al.* Phys. Rev. Lett. 87, 127201 (2001)]

Surface core level shift used as a tool to identify PdMn systems on Pd(100)

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Surface and interface core level shifts (CLS) of Pd $3d_{5/2}$ is calculated *ab initio* for the 1 ML Mn/Pd(100) system, as well as for three possible structures of reconstructed surface that may appear after annealing of the above system. The results are then compared to a recent experimental study by A. Sandell *et al.* (PRB **65**, 035410 (2001)). The calculations are carried out in the framework of the interfaces KKR-ASA (CPA) Green's function method. The shifts are calculated according to the complete screening picture which includes both initial state (electron energy eigenvalue) and final state effects (relaxation of the core-hole) in the same scheme. The effect of different types of magnetic ordering, ferromagnetic or anti-ferromagnetic, on the CLS of the as deposited and reconstructed samples was considered. From a comparison of calculated

CLS with experiment, we identify which structure is actually present in experimental samples. Our conclusions agree with the work of A. Sandell *et al.*, and point towards the same structure after annealing. We conclude that theoretical calculations of CLS provide a reliable tool for the solution of nonequilibrium structures at surfaces and interfaces.

Multiple-scattering theoretical approach to scanning tunneling spectroscopy

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The qualitative and quantitative theoretical description of scanning tunneling spectroscopy (STS) is usually based on the popular Tersoff-Hamann model. By simply relating the tunneling current to the spectral density of the sample, however, relevant properties of the tunneling through the tip-sample system are neglected.

Viewing electronic tunneling as a scattering process, we present a formulation of STS in terms of multiple-scattering theory which takes into account the tip-sample interaction. Further, electronic properties of the constituent systems can be obtained by ab-initio calculations. Besides a presentation of the general formalism and its implementation in a spin-polarised relativistic layer-KKR scheme, we sketch results for prototypical systems, with a focus on features of the scattering-theoretical approach.

Half-ferromagnetism and Slater-Pauling behavior in the Heusler alloys

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The development of magnetoelectronics has increased the interest in materials which can enhance the performance of spin-dependent devices. Such materials are the so-called half-metals which present a gap in the minority band resulting in 100% spin-polarization at the Fermi level. A significant number of the intermetallic Heusler alloys have been predicted to be half-metals. In this contribution we will present a complete study of both the bulk and surface properties of such Heusler alloys including both the families of the so-called half-Heusler alloys like NiMnSb and of the full-Heusler alloys like Co_2MnGe. Based on the *ab-initio* results for these compounds we will discuss the origin of the gap which is fundamental for the understanding of their electronic and magnetic properties. We will show that for both families of compounds the total spin magnetic moment M_t scales with the number of valence electron Z_t, such that $M_t = Z_t - 18$ for the half-Heusler and $M_t = Z_t - 24$ for the full-Heusler alloys, thus opening the way to engineer new half-ferromagnetic Heusler alloys with the desired magnetic properties. Although the surfaces loose in-general the half-ferromagnetic character and exhibit a small degree of spin-polarization, we will show that in the case of compounds containing Cr, the large enhancement of the Cr moments at the surface reduces the effect of the surface states and leads to a very high spin-polarization of the surfaces, *e.g.* 84% for the CrAl-terminated $Co_2CrAl(001)$ surface or even 100% for the Cr-terminated CrAs(001) surface, so that these compounds might be promising for spindependent devices.

Electronic and magnetic properties of ferromagnet/semiconductor interfaces

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The electronic and magnetic properties of ferromagnet-semiconductor heterostructure systems have been studied using the scalar-relativistic KKR-CPA and fully-relativistic TB-KKR band structure methods. Concerning the resulting magnetisation profiles of multilayer and trilayer (FM/SC/FM) systems the most important features are that no magnetically dead layers occurred and an appreciable induced magnetisation was found in the semiconductor subsystem. Interdiffusion doesn't lead to magnetically dead layers in the FM-layer and is energetically unfavourable. Investigating the hyperfine interaction and the magnetic circular dichroism (MCXD) more detailed information on the electronic structure could be obtained. Calculations of the interlayer coupling energy show interesting behaviour dependent on the thickness of the SC layer. Similar to metallic multilayer systems it could be shown that the magneto-crystalline anisotropy correlates with the anisotropy of the orbital moment.

The work has been based so far on unrelaxed ferromagnet-semiconductor heterostructures. In the near future investigations on the influence of lattice relaxations and interface reconstructions will be one of the issues of the project.

Relativistic Effects in the Transport Properties of Ferromagnetic-Semiconductor-Ferromagnetic (FM/SC/FM) Trilayer Systems

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Spin-dependent transport between two ferromagnetic electrodes separated by either an insulator or a semiconductor has received a lot of interest in the last years due to its potential technological applications. Recently it could be shown that a measurable spin-polarised injection can be obtained in a TMR Fe/GaAs diode even at room temperature.

Many theoretical studies devoted to TMR systems can be found in the literature, but they either neglect relativistic effects or treat the crystalline structure in an approximate way. To allow for a most general description, our present investigations on FM/SC/FM systems have been performed within the framework of Tight-Binding Spin-Polarised Relativistic Multiple Scattering Theory (TB-SPR-KKR). The electronic structure and magnetic properties of Fe/GaAs/Fe as a representative example will be presented.

The transport properties of this systems are investigated by means of the Landauer-Büttiker formalism. The tunneling conductance and the TMR are calculated on a relativistic level. Model

calculations allow us to gradually manipulate the strength of the spin-orbit coupling SOC and to investigate in detail its quantitative and qualitative influence on the spin-dependent transport.

Probing magnetic susceptibilities using the field-induced magnetic circular dichroism

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The magnetic circular dichroism in X-ray absorption (MCXD) is now a standard tool to probe the spin and orbital moments in magnetic materials by exploiting the so-called sum rules. In these systems the magnetic dichroism may be ascribed to the spontaneous exchange splitting. On the other hand, it its known that the magneto-optical Faraday effect, for example, can be observed for magnetic materials as well as for non-magnetic materials if they are exposed to a magnetic field. Accordingly, magnetic circular dichroism in X-ray absorption should be observable also in non-magnetic materials exposed to a magnetic field. A theoretical description of such an experiment is presented that is based on a combination of a fully relativistic linear response formalism and a corresponding treatment of magnetic circular dichroism. It is demonstrated that application of the magnetic sum rules now gives access to the spin and orbital element projected susceptibility of the system under investigation. In particular one finds that it is only the VanVleck contribution to the orbital susceptibility that is probed. In contrast to spontaneously magnetized systems, however, there are orbital contributions derived from the dichroic signal that stem from the external field and also from the intrinsic spin-orbit coupling. Illustrating examples will be presented for various transition metal systems that will demonstrate the usefulness and applicability of the new approach.

Disorder-induced magnetism in $TiFe_xCo_{1-x}$

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The transition metal system $TiFe_xCo_{1-x}$ has a CsCl-structure with Ti on one sublattice and a random distribution of Fe and Co according to the concentration on the other sublattice. From previous experimental investigations it was concluded that if this quasiordered structure is formed, $TiFe_xCo_{1-x}$ is in a paramagnetic state. Only if a small numbers of Fe or Co atoms (1-2%) are occupying Ti sites (so called anti-sites) the alloy system gets a weak itinerant ferromagnet for $0.2 \leq x \leq 0.8$. To investigate this interesting disorder-induced magnetisation in more detail, we have used the Korringa-Kohn-Rostoker(KKR) band structure method. The disorder in the system has been accounted for by means of the Coherent Potential Approximation(CPA). Our calculations demonstrated that $TiFe_xCo_{1-x}$ is indeed paramagnetic for all concentrations x if these is no mixing of the two sublattices. Only a small mixing on the other hand gives rise to the formation of a spontaneous magnetisation that is in fairly good agreement with experiment.

Our calculations give also a simple explanation for the puzzling Fe-Mößbauer data. While the Fe atoms on anti-sites have a large moment and hyperfine field, the hyperfine field of Fe-atoms on proper sites are very small because the valence band and core polarisation contributions nearly cancel another.

LMTO Green Function approach for the *ab initio* calculation of the optical and magnetooptical properties of solids.

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An approach for the calculations of the optical and magnetooptical properties of solids based on the one-particle Green Function introduced by Huhne and Ebert [1] and Szunyogh and Weinberger [2] is applied in the framework of the LMTO method. An advantage of the energy independent basis functions is explicitly taken into account which gives rise to the incredible acceleration of the calculations in comparison with the standard KKR scheme. At the same time the approach keeps all advantages of the more accurate KKR scheme as the possibility to account both for many-body effects and disorder effects in terms of the nonlocal energy dependent self energy. Preliminary results based on the simplified method of the Brillouin zone integration shows reasonably good coincidence with the standard methods for optical calculations based on the wave function formalism for Fe and Ni.

[1] T. Huhne and H. Ebert, *Phys. Rev. B* **60**, 12982 (1999).
[2] L. Szunyogh and P. Weinberger, *J. Phys.: Condensed Matter* **11**, 10451 (1999)

Electron-electron interaction viewed by one-photon two-electron excitations

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Theoretical and experimental evidence is provided that the spectrum of a photoexcited electron pair carries detailed information on the electron-electron interaction in metals. The theory is based on a two-particle LKKR approach that will be presented at the meeting. The main features found in the two-particle spectra have been assigned to (a) the exchange-correlation interaction, (b) the electronic band structure, (c) the photoelectron diffraction, and (d) the specific experimental setup. Comparison with experiments is made and common features and differences to the atomic case are pointed out.

Magnetization of the unsegregated and segregated (100) surface of MoV binary alloy

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Using *ab initio* total energy calculations in conjuction with statistical Monte Carlo simulations we have investigated magnetic properties of the (100) surface of the $Mo_{25}V_{75}$, $Mo_{50}V_{50}$ and $Mo_{75}V_{25}$ binary alloys both for homogeneous concentration profile and in the presence of surface segregations. While the MoV alloy is not magnetic in bulk in the whole range of concentrations, we predict a noticeable magnetization to occur at the top layer of the (100) surface. The surface segregations essentially enchance surface magnetization for Mo-rich alloys, so the average atomic magnetic moment is three times larger at the segregated surface in comparison with the homogeneous one. In order to find out an origin of the surface magnetization we have analyzed the alloy electronic structure.

First-principle study of the magnetoresistance effects in magnetic nanocontacts

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We present ab-initio calculations of the transport properties of the metallic atomic-sized nanocontacts. The nanocontacts were modeled by atomic chains of Co, Fe, Cu, Si, Al separating two semi-infinite magnetic Co-leads. We used the first-principle screened Korrigna-Kohn-Rostoker method to calculate the electronic properties of the systems, treating the Co leads and atomic chains on the same footing without any model parameters. The Landauer formalism was applied to investigate the conductance and magnetoresitance (MR). We found MR ratios of about 20-30

PHASE SEPARATION AT INTERFACES IN $La_{2/3}Ca_{1/3}MnO_3$

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Mixed-valence manganites are oxides with perovskite structure and general formula $A_xA'_{(1-x)}MnO_3$. They show a large number of properties originating from the many competing interactions between spin, charge and lattice. Therefore, they are very sensitive to structural modifications and to changes in the doping value, which can induce transitions from a magnetoelectronic phase to

another. Among manganites, several compounds are half metallic ferromagnets whose high spin polarization is interesting for spintronics devices. For instance, very large magnetoresistance (MR) ratios are obtained in tunnel junctions at low temperature. However, the temperature dependence of the MR which decays much faster than magnetization and has prevented the observation of MR signal at room temperature so far. The precise cause of this behavior is unknown even if several studies suggest that it could be due to a loss of polarization at interfaces. Here, we report on magnetotransport and ^{55}Mn NMR measurements of thin films of $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) grown on $SrTiO_3$ (STO) and on $NdGaO_3$ (NGO) substrates, and on ceramic powders of $La_{2/3}Ca_{1/3}MnO_3$ with different grain sizes. Two lines are detected in the NMR spectra, indicating the presence of two types of regions with different conductivities. The detailed analysis of the data indicate that low-conductivity regions are more prominently located close to surfaces and interfaces. These data bring new elements for the understanding of the temperature decay of the MR of tunnel junctions and for the design of better manganite/insulator interfaces. Besides, the observation of parasite electronic phases close to surfaces or interfaces in $La_{2/3}Ca_{1/3}MnO_3$, a homogeneous compound in its bulk form, confirms the theoretical prediction of disorder-promoted phase separation.

Magnetic nanostructures on metal surfaces

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Magnetism, structure and interactions on the atomic scale are discussed. We present ab initio results on interatomic interactions between magnetic adatoms on a metal surface. We concentrate on Co adatoms and clusters on Cu(111) and Cu(100) surfaces. The scattering of surface state electrons by the Co adatoms on Cu(111) surface is studied by means of ab initio multiple-scattering KKR Green's function method. The quantum interference between incident and scattered surface state electrons leads to standing waves in the electronic density around adatoms. Calculations resolve the lateral oscillations of the local density of states with a wavelength expected from the surface state band structure. Substrate-mediated long-range oscillatory interaction between adatoms is determined. Experimentally the direct observation of long-range interaction between adatoms up to 60 Angstrom distance is performed using pair correlations of diffusing adatoms recorded with a low temperature STM. The measured long-range interaction energies are in very good agreement with ab initio calculations.

Atomic relaxations in magnetic clusters are performed using ab initio based many body potentials constructed for a low-dimensional systems. Our results lead to the conclusion that the size-dependent mesoscopic mismatch, rather than the macroscopic one, is the driving force for strain-relieving effects at the mesoscale. The strain relief is predicted to have a profound effect on the shape of islands. Strain relaxation in Co islands leads to a reduced stress contribution in the partially filled layers. The stress in Co monolayers has been measured during epitaxial

growth on Cu(001). The Co-induced stress is found to oscillate with a period of one atomic layer. Our experiments and atomic scale calculations ascribe the stress variation to the relaxation of epitaxial mesoscopic misfit strain in the islands.

The influence of hydrogen adsorption on magnetic properties of Ni/Cu(100) surface

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Ni/Cu(001) is known as a unique system showing the spin-reorientation transition (SRT) from an in-plane to out-of-plane magnetization direction when the Ni-overlayer thickness is increased. Recent experiments demonstrate that the critical thickness of the magnetization direction switching is strongly reduced by the H_2 adsorption. Here, the relaxed multilayer-structures have been investigated by the self-consistent all-electron full-potential linearized augmented plane-wave method (FP-LAPW). The relaxed geometries, determined by total energy and atomic force calculations, show that H-monolayer (ML) strongly influences the interlayer distance between the Ni-surface and sub-surface layers yielding the outward relaxation of Ni-layer at H/Ni interface. Furthermore, a large decrease of local magnetic moments in the top surface area has been found if the surface was covered by H. Moreover, we present an *ab-initio* investigation of SRT. As a structural model we use the free-standing Ni-films and symmetric Ni/Cu/Ni-films covered by ML of H-atoms. Second, we calculate the magneto-crystalline anisotropy energy (MAE) employing the "magnetic force" theorem for the magnetization rotation. For fully relaxed Ni-films the SRT critical thickness of 4 ML is found in good quantitative agreement with the experiment. It is mainly caused by the reduction of Ni-film surface MAE due to the H-adlayer. Finally, we analyse the element specific contributions to the MAE using its relation with the anisotropy of the orbital magnetic moment.

Giant Magnetoresistance in carbon nanotubes

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(CN's) are seamless graphitic cylinders [1] with electronic properties which are sensitively related to their geometry. Spin-polarized transport in nanotubes is of a great interest since CN's could play a role in future nanometer-scale electronic devices. We have studied Giant Magnetoresistance (GMR) in carbon nanotubes using the Landauer-Büttiker formula to calculate the differential quantum conductance and the GMR ratio for metallic and semiconducting carbon nanotubes. We consider two ferromagnetic regions with magnetization perpendicular to the tube axis, in contact with a non-magnetic finite-length nanotube. We calculate the change in conductance and hence the GMR ratio arising when the orientation of the magnetic moments

changes from parallel to antiparallel. The Hamiltonian of our system is a parameterised four-state (s, p_x, p_y, p_z) Hamiltonian based on a global fit to density functional results for graphite, diamond and C_2 [2]. In order to calculate the conductance we use a general Greenś function scattering technique [3]. The effects of a structural twist and a double barrier on GMR are studied and depending on the position of the Fermi energy, GMR ratios in excess of 200% are predicted.

[1] S. Iijima, *Nature* (London)**354**, 56 (1991)

[2] D. Tománek,M. A. Schluter, *Phys. Rev. Lett.* **67**,2331 (1991)

[3] S. Sanvito, C. J. Lambert, J. H. Jefferson and A. M. Bratkovsky, *Phys. Rev. B* **59**, 11936 (1999)

Relativistic calculation of spin-wave spectra in thin magnetic films

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We have formulated a relativistic treatment to calculate the low energy magnetic excitation spectrum of thin magnetic films. The method can be considered as a relativistic generalization of the well known torque method by Lichtenstein et al. [1], however, the mapping of the energy of the system onto a Heisenberg model is avoided. Our method can also supply well-defined layer resolved magnetic anisotropies. The method is demonstrated for ultrathin Fe films on Cu(100) and Au(100) surfaces as cases for an out-of-plane ground-state magnetization, while also for Co films on Cu(100) with an in-plane magnetization. The effect of the spin-orbit coupling can be seen, in particular, by inducing a gap in the long wavelength part of the magnon spectra and resulting in a clear difference in the spectrum along the (100) and (010) directions for the in-plane magnetized Co/Cu(100) system.

[1] A.I. Lichtenstein, M.I. Katsnelson, V.P. Antropov, and V.A. Gubanov, *JMMM* **67**, 65-74 (1987)

Exchange interactions in magnetically frustrated systems

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Recent *ab initio* calculations of volume dependences of magnetic properties for the most typical Invar system, a random fcc Fe-Ni Invar alloy, have shown that the evolution of the magnetic structure already at zero temperature is characterized principally by a continuous transition from the high-spin ferromagnetic state at high volumes to a disordered noncollinear configuration at

low volumes [1]. This indicates the existence of large number of magnetic states in the system separated from each other by very small energy differences. Thus, the magnetic state in the system is highly frustrated. In this work we calculate from the first-principles [2] parameters of the classical Hiesenberg Hamiltonian for magnetic interactions in pure fcc Fe and fcc Fe-Ni alloys, the pair exchange parameters J_{ij}, as well as the effective exchange parameter J_0. We find that in pure Fe J_0 is almost completely dominated by J_{ij} between nearest neighbors. We also show that there exists a particular area of volumes where more distant pair exchange parameters are big, of the order of J_{ij} between the first nearest neighbors, but their contributions to the effective exchange parameter cancel each other almost exactly due to oscillating signs of these interactions. However, this peculiar behavior of exchange integrals disappears almost completely at Invar concentrations in Fe-Ni alloys. The origin of magnetic frustrations in random alloys is identified and discussed.

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3.2 RTN1 Workshop Announcements

3.2.1 Workshop on Spin Mesoscopics

EU RTN "Computational Magnetoelectronics"
NEDO "NanoMagnetoElectronics" network
ESF Working Group "Magneto-Electronics"
joint workshop on
"Spin Mesoscopics"

on the campus of the University of Twente,
Enschede
The Netherlands

March 15th - March 17th, 2003

Scope: The workshop will cover spin-transport in general (including materials) but with particular emphasis on developments driven by shrinking the size of devices such as MRAMs.

Arrival: Friday evening, March 14th, 2003

Departure: Monday afternoon, March 17th, 2003

Programme: We plan to have about 10 longer invited presentations, and about 20 shorter contributed oral presentations, the selection being based upon the abstracts we receive. In addition, there will be the possibility to hang up a poster in the meeting room for the duration of the meeting. In the evening there will be interactive sessions based on one-sheet presentations.

Accomodation: on Campus in the Conference Hotel "Drienerburght" or in guesthouse "Logica".

Deadlines:
Registration: 17th January 2003
Submission of Abstracts: 17th January 2003
Submission of titles for one-sheet presentations: 10th March

More information can be found on the workshop website which will be updated regularly.

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

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4 News from the new RTN2 and RTN3 Networks ("f-electrons" and "Exciting")

"Ab-initio Computation of Electronic Properties of f-electron Materials" (f-electrons)

and

"Optical Properties of Solids" (Exciting)

4.1 RTN2 and RTN3 Position Announcements

POST-DOCTORAL POSITION

Materials Design

Le Mans, France

A post-doctoral position is available at Materials Design in Le Mans, France within the European Research and Training Network "Ab-initio Computation of Electronic Properties of f-electron Materials". The research will focus on the optical properties of materials containing rare earth elements, such as the red pigment cerium sulfide. The candidate is expected to have experience in electronic structure methods, should be younger than 35 years, and should be a national of a Member State of the European Community (other than France) or of an Associated State or residing in the Community for at least five years prior to the present appointment.

Applications should be sent by email to

Erich Wimmer
ewimmer@materialsdesign.com

DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF AARHUS, DENMARK

Two Post-doctoral Positions

Condensed Matter Theory: Electronic Structure of f-electron Materials or Optical Properties of Solids

Applications are invited for two post-doctoral positions funded by the European Research Training Networks, **Psi-k f-electron**: '*Ab-initio Computation of Electronic Properties of f-electron Materials*' and **EXCITING**: '*First-Principles Approach to the Calculation of Optical Properties of Solids*', respectively.

The positions are available for a period of 2 years starting first half of 2003. Extension is possible.

The applicants must comply with the RTN rules for network employment of young scientists: The applicants should hold a Ph.D. degree or equivalent in Physics or Chemistry, be aged 35 or younger, and should have some experience in computational Condensed Matter Theory. They must be of European Union nationality, or from one of the Associated Nations, or have resided in an EU country for the last five years or longer. Danish citizens are excluded, however.

The successful applicants shall participate in either of the above network projects. This implies applications of present computer codes to solid systems of high current interest as well as development of improved computer codes. The projects are collaborations in international teams and some travel activity between the research centers involved must be foreseen. More detailed information concerning the project can be obtained upon request.

Applicants must submit a curriculum vitae, a description of scientific accomplishments, and a list of publications (all in 4 copies), and 3 copies of publications to be considered in the evaluation.

The Faculty refers to the Ministerial Order No. 820 of 31.8.2000 on the appointment of teaching and research staff at the universities under the Ministry of Research and Information Technology.

Salary as agreed between the Danish Ministry of Finance and the Confederation of Professional Unions.

Applications should be addressed to

The Faculty of Science,
University of Aarhus, Ny Munkegade, Building 520,
DK-8000 Aarhus C, Denmark

and marked 212/5-27.

The deadline for receipt of all applications material is December 16th, at 12,00 noon.

For further information, contact

Dr. A. Svane or Prof. N. E. Christensen,
Department of Physics and Astronomy,
University of Aarhus, Ny Munkegade,
DK-8000 Aarhus, Denmark

Phone: (+45) 8942-3678, 8942-3666,
Fax.: (+45) 8612-0740,
Email: svane@phys.au.dk or nec@phys.au.dk

Information about the Department can also be found on http://www.phys.au.dk.

Postdoc Position
in Theoretical Solid State Physics
at IFW Dresden

We would like to announce an open postdoc position in the framework of the European Research Training Network

"Ab-initio Computation of Electronic Properties of f-Electron Materials."

The applicant should be a non-German citizen of the European Community or an associated state and should not have worked in Germany for more than 12 months during the last two years. (The precise regulations are found at `http://www.cordis.lu/improving/networks/faq.htm#q5` .)

The project, to be carried out at IFW Dresden (http://www.ifw-dresden.de) in cooperation with 7 other network partners in Europe and USA, includes

(1) density functional studies of surface magnetism on lanthanide elements and compounds, using the recently developed FPLO code (http://www.ifw-dresden.de/FPLO/);

(2) code development with respect to surface-specific properties and tasks.

Close contact with related experimental work at IFW Dresden, University of Technology Dresden (http://www.tu-dresden.de), and the Max-Planck Institute for the Chemical Physics of Solids Dresden (http://www.cpfs.mpg.de) is envisaged, as well as collaboration with several Dresden groups active in solid state theory.

The applicant should preferably have a safe background in solid state physics, good knowledge of density functional theory, and experience in the understanding and development of extended code for numerical purposes (FORTRAN 90 and/or C).

We offer a one-year position, extendable up to 3 years, at the level BAT IIa-O (annual net income about 20 kEUR, depending on age and family status), as well as relocation and regular travel costs to the home scientific community of 7 kEUR in total.

The Department of Theoretical Solid State Physics at IFW Dresden consists of eleven PhDs in solid state theory, three PhD students, and several guest scientists, see

http://www.ifw-dresden.de/agtheo/eagtheo1.htm.

The group has up-to-date computer facilities, daily coffee meetings, and a lively exchange with a number of other groups inside and outside of Dresden (theoretical and experimental, physics

and chemistry). The city of Dresden is situated mid-way between Berlin and Prague, in the valley of river Elbe. With a population of about 500,000, it is known for a rich cultural live and for its baroque silhouette.

Interested candidates should send their application together with a curriculum vitae, a list of publications or current research activities, and other relevant material to:

Dr. Manuel Richter
Dept. of Theoretical Solid State Physics
IFW Dresden e.V.
P.O. Box 270016
D-01171 Dresden, Germany

Email: m.richter@ifw-dresden.de

4.2 RTN2 and RTN3 Workshop Announcements

4.2.1 Workshop Hands-on-FPLO

March 28 - April 1, 2003, in Dresden

Supported by:

- European Commission (RTN Psi-k f-electron)
- IFW Dresden e.V.

Purpose:

- Introduction into the concept, the code, and the handling of the FPLO package
- Exchange of experience among the users

Organizers:

- Helmut Eschrig: h.eschrig@ifw-dresden.de
- Klaus Koepernik: k.koepernik@ifw-dresden.de
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Content:

The FPLO package is a full-potential local-orbital minimum-basis code [1] to solve the Kohn-Sham equations on a regular lattice using the local spin density approximation (LSDA). The

situation of a chemically disordered structure is covered by a CPA solver [2], relativistic effects can be treated in a related 4-component code [3], and the LSDA+U formalism is implemented. Much effort has been spent to achieve a level of numerical accuracy which is comparable to advanced full-potential LAPW implementations, though the basis set is one order of magnitude smaller. In particular, the **absolute** values of the total energy agree with the results of WIEN-97 within about 1 mHartree per atom [1]. WIENxx and FPLO are to a certain extent complementary. While WIENxx in most cases still sets the accuracy standard, a major advantage of the FPLO package is its minimum basis concept. It makes highly accurate full-potential calculations for elementary cells of up to 100 transition metal atoms feasible and is a good starting point for approaches beyond the LSDA.
FPLO-2, including the scalar relativistic LSDA version of FPLO, has been released at the first workshop in March 2002. FPLO-3, to be released at the announced workshop, will include the possibility to treat chemical disorder within the coherent potential approximation (CPA) and the LSDA+U approach. Moreover, its performance, reliability, and requested main storage have been further optimized.

References:
[1] K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999); I. Opahle, K. Koepernik, and H. Eschrig, Phys. Rev. B 60, 14035 (1999).
[2] K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig, Phys. Rev. B 55, 5717 (1997).
[3] I. Opahle, PhD thesis, TU Dresden 2001.

Participants:
Those who are interested to get and use FPLO-3. Active users of the code are welcome as well to exchange their experience with other users and to become aquainted with the new features of FPLO. For capacity reasons (available terminals and tutors in the practical sessions) we will have to restrict the number of participants to about 20. The workshop will primarily be a tutorial one. It should enable the participants to use FPLO-3, to interprete its output quantities, and to cope with simple problems that may arise when using the code.

Place:
Room D2E.27, IFW Dresden e.V., Helmholtzstr. 20, Dresden, Germany
http://www.ifw-dresden.de

Time:
March 28 - April 1, 2003.
The workshop will start immediately after the annual meeting of the German Physical Society (Solid State Physics).

Fees:
The workshop fee amounts to **EUR 100**. Students may register at a reduced fee of **EUR 50**. These fees include the participation in all lectures and exercises, lecture materials, the get-together reception, lunch and coffee during the workshop. **Not included** are any accomodation

costs or license fees.
Members of the RTN Psi-k f-electron may participate free of charge.

Accomodation:
The accomodation should be arranged by the participants. We have optionally reserved 10 single rooms at the City-Herberge Dresden (EUR 31.50 per night, including breakfast). The option is valid till February 28, 2003. You can make your reservation at the City-Herberge Dresden via the internet, http://www.city-herberge.de. Please quote "pre-reservation by IFW/Workshop". If you prefer another accomodation, you will easily find a number of good hotels close to the center of Dresden. Please contact the organizers, if you need assistance.

Pre-registration
Please send, as early as possible, an email to Manuel Richter (m.richter@ifw-dresden.de) giving your name, address, and probablility of participation.

Registration:
Please pay the registration fee, free of any bank charges, **before February 15** to the following account and confirm your participation by email:

Name of bank	Deutsche Bank AG
Address of bank	Glacisstr. 2, D-01099 Dresden
Bank account no.	53 53 131 00
Sort code no.	870 700 00
SWIFT code	DEUT DE 8C
Payment reference	IFW-Dresden
NUIM reference	76 005 05 1

Schedule

Friday, March 28
14:00 Registration
15:00 Opening (Helmut Eschrig)
15:05 DFT and the FPLO idea (Helmut Eschrig)
16:30 Coffee
17:00 The FPLO concept (Klaus Koepernik)
18:30 Explanation of licence conditions (Manuel Richter)
19:00-21:00 Get-together reception

Saturday, March 29
9:00 Installation of FPLO-3 (Ulrike Nitzsche)
9:30 Exercise: How can I run FPLO-3 on simple systems (Manuel Richter)
11:00 Coffee
11:30 Fixed spin-moment calculations and contact hyperfine fields (Michael Kuz'min)

12:30 Application to complex structures (Helge Rosner)
13:00 Lunch
14:00 Exercise: Fixed spin-moment (Michael Kuz'min)
15:40 Coffee
16:00 Performance and parallelization (Ulrike Nitzsche)
17:00 WIEN and FPLO: a comparison (Martin Divis)
17:30 Private discussion and exercises on request

Sunday, March 30
9:00 Coherent Potential Approximation in FPLO (Klaus Koepernik)
10:30 Coffee
11:00 Exercise: Coherent Potential Approximation (Klaus Koepernik)
12:20 Supercell approach for surfaces (Manuel Richter)
13:00 Lunch
14:00 How to extract model parameters from FPLO (Helge Rosner)
15:00 Coffee
15:30 Exercise: Model parameters (Helge Rosner)
16:30 Application to antiferromagnetic systems (Stefaan Cottenier)
17:00 Geometry optimization with several free parameters (Denis Mertz)
17:30 Private discussion and exercises on request

Monday, March 31
9:00 LSDA+U in FPLO (Klaus Koepernik)
10:30 Coffee
11:00 Exercise: LSDA+U (Igor Chaplygin)
12:20 Summary of new features of FPLO-3 (Klaus Koepernik)
13:00 Lunch
14:00 Relativistic FPLO (Ingo Opahle)
15:30 Coffee
16:00 lo-WIEN and RFPLO: a comparison (Pavel Novak)
16:30 Private discussion and exercises on request

Tuesday, April 1
Departure

5 News from the ESF Programme

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

5.1 Reports on ESF Workshops/Conferences

5.1.1 Report on Swedish Summer School on Magnetism

5-9 July, 2002
by Olivier Bengone and Olle Eriksson

Summary of workshop

A total of 50 participants from 10 countries attended the workshop from 5-9 July 2002. 20 lectures covered a wide range of topics from technical details in spin electronics and electronic structure methods to more practical aspects of magnetic sensor technology and information storage. The format of the summerschool was educational and didactic, where the basic aspects of the different questions were addressed. The different backgrounds of the participants and the lecturers (experimental physics, theoretical physics, industrial) allowed substantial cross breeding that is fruitful. The lively discussions revealed a high level of activity in this field. The summerschool embraced the following topics.

Experimental aspects of thin film magnetism

This topic was covered by Profs.Hartmut Zabel, Björgvin Hjörvarsson, Panagiotiotis Poulopoulos, Janusz Sadowski, Lars Samuelson and Dimitri Arvantits. Experimental techniques for thin film growth and characterisation were discussed. In addition several experimental techniques for probing magnetic properties, such as neutron scattering, XMCD, MOKE etc. were described and ample of examples of such investigations, especially for thin film systems, were given. In addition Prof. J.Kirschner described extremely delicate measurements of surface magneto-striction and Prof. J.Schoenes lectured on expeirmental and theoretical aspects of magneto optics.

Spin electronics and spin transport

Various aspects of spin electronics were discussed by Prof. M.Tsoi, A. Fert, N. Garcia, and F. Nguyen-van Dau. Experimental problems with spin injection were discussed as well as current induced excitations of spin waves and ballistic magneto-resistance in nano-contacts. In addition

several possible applications of spin-electronics were described.

Theory

Theoretical aspects of thin film magnetism, exchange interactions in general, electronic structure theory and its applications to thin films and magnetism were discussed by Prof. S. Blugel, S. Mirbt, M. Brooks, I. Sandalov and M. Katsnelson. In particular phenomena such as CMR and GMR were discussed, spin polarised transport in general as well as improvements to the density functionals normally used. The dynamical mean field approximation was introduced by Prof. Katsnelson.

Industrial aspects

A very illuminating talk on industrial aspects of spin electronics, spin polarised transport, information technology etc. was given by Dr. O. Heinonen, Seagate. Future, possible directions of this field was discussed with emphasis on both technical and finacial aspects. Technical, industrial aspects of spintronics was also covered by Prof. Nguyen-van Dau.

Conclusions

The summerschool was a great success, with a high scientific and didactic level from all the lecturers. The popularity of this workshop and the intense interest in this research field suggest that another symposium should be held on this topic within the next 1-2 years.

Participating students and post docs

Olla Wessley
Arantxa Fraile Rodriguez
Alexei Grechnev
Emma Kerr
Steven Watts
Matts Björck
Cecilia Andersson
Carlos Ortiz
Eoin Clifford
Till Burkert
Olle Eriksson
Raquel Lizárraga
Anna Maria Blixt
Thomas Dziekan
Björn Skubic

Erik Holmström
Anders Bergman
Andreas Kissavos
Weine Olovsson
Lars Bergqvist
Biplab Sanyal
Welimir Meded
Saeed Kamali
Gabriella Anderson
Petros Souvatzis
Sa Li
Helmut Rathgen

Abstracts of the invited talks

- **Experimental methods of thin film magnetism**
  Hartmut Zabel

  Bochum

  Experimental methods are discussed to analyze the magnetism of thin films, such as the magnetic hysteresis, the magnetic anisotropy, and magnetization profile, the magnetic domain structure, and magnetic phase transitions. One of the most important techniques is the magneto-optic Kerr effect. This effect has many different facets, which enable to explore the vector magnetism of thin films up to the penetration depth of light. In contrast, neutron reflectivity which will also be discussed, adds structural information to the magnetic analysis, resulting in a layer-wise vector-magnetometry. Polarized neutron reflectometry is indispensible for the analysis of non-collinear spin structures in magnetic multilayers.

- **Excitation of spin waves by an electric current**
  Maxim Tsoi

  IBM Almaden Research Center, San Jose, California

  Spin waves, or magnons, are intrinsic excitations in magnetic materials and have attracted considerable attention since introduced by Bloch in 1930 [1]. Recently ideas of spintronics have impacted this field dramatically. Slonczewski [2] and Berger [3] introduced completely new aspects of the physics of metallic ferromagnets in the presence of an electric current of high density. Excitation of magnons by an electric current has been predicted [2-4] and seen in magnetic multilayers [5-8], where the

driving force for the excitations is the spin-momentum transfer associated with an electric current flow. We have developed a microcontact technique (magnetic microcontact spectroscopy) to investigate the current-driven magnon generation [5,9]. It was shown that injection via a point contact of a sufficiently large current density into a magnetic multilayer produces a step increase in the resistance of the multilayer [5-8]. This observation represented indirect evidence of the excitation of high-frequency magnons by an electric current previously predicted by Berger and Slonczewski. We have now more fully tested the prediction by directly detecting electromagnetic waves radiated by these current-driven magnons [9]. In this talk I will show that irradiation of a point contact by external microwave radiation directly shows the high-frequency nature and at least partial phase coherence of such current-induced excitations. The technique provides detailed information on the spectrum of current-driven magnons. Our results suggest the potential of high frequency applications, such as a monodomain sub-micron-scaled oscillator powered and tuned by an applied current, while our observation of emission of coherent current-driven magnons stimulated by an external radiation of the same frequency supports the feasibility of a spin-wave maser SWASER (spin-wave amplification by stimulated emission of radiation). Some further interesting applications of the technique, particularly, for studying fluctuation phenomena, resonant magnon generation, acoustic wave generation, etc., will be presented. For instance, I will describe complex variations in resistance of a Co/Cu multilayer, generated by injection of an adjustable dc current density via a point contact [10]. We attribute these variations to coupling of current-induced spin waves to lattice vibrations, leading especially to current-driven resonant excitations of phonons. *Indispensable contributions of A. G. M. Jansen, J. Bass, V. Tsoi, and P. Wyder to this work are gratefully acknowledged.

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[8] E. B. Myers, D. C. Ralph, J. A. Katine, R. N. Louie, and R. A. Buhrman, Science 285, 867 (1999).

[9] M. Tsoi et al., Nature 406, 46 (2000)

[10] M. Tsoi, et al., to be published.

- **Spin injection : fundamentals, injection into semiconductors, spin transfer**

Albert Fert

Unit Mixte de Physique, CNRS-THALES and Universit Paris-Sud, Orsay, France

Spin injection is involved in many aspects of nowadays spin electronics. I will first present the fundamental physics of spin injection and spin accumulation at the interface between magnetic and nonmagnetic semiconductors. Then I will focus on two important topics: 1)Injection of spins from a ferromagnetic metal into a semiconductor (possible with a well adapted tunnel resistance). 2)Magnetization reversal by spin injection and spin transfer.

- **Quantum-dot physics, an experimental overview**
  Lars Samuelson

  Lund University, Sweden

  I will give an overview of the experimental situation concerning quantum-dot physics.

- **Thin film magnetostriction**
  Jürgen Kirschner

  Halle University, Germany

  In this lecture, I will give an introduction to the field of thin film magnetostriction.

- **Theory of thin film magnetism**
  Stefan Blügel

  Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

  I will review the present understanding of itinerant magnetism with the emphasis on surfaces and ultra-thin films. I will discuss within the Stoner model for ferromagnetism and antiferromagnetism the role of the coordination number or dimensionality for the magnetism in low dimensions. Non-collinear magnetism is introduced and the mapping to the Heisenberg model in order to give access to finite temperature magnetism and the search for complex magnetic ground states is discussed. Antiferromagnets on a triangular lattice is investigated as a case study. Systematic ab-initio calculations for a wide range of systems are shown which give a quantitative verification of the general discussions presented.

- **Ballistic Magnetoresitence Results in Atomic and Nanometer Size Magnetic Contacts**

Nicolas García

Laboratorio de Física de Sistemas Pequeños y Nanotecnología (CSIC) Serrano 144 Madrid 28006, Spain

In this talk I will review the recent results on ballistic magnetoresistance (BMR) in magnetic nanocontacts obtained in our lab and in many others around the world. I will look at atomic contacts as well as to electrodeposited Ni- Ni nanocontacts where very large BMR have been obtained in 10-30nm section electrodeposited nanocontacts. This very large effect maybe due to a dead magnetic layer, containing O, Cl, S or whatever element, that filters adequately the electrons of Ni producing a electric current with full polarization. The physical explanation is explained by the theory of domain wall scattering at the nanocontact of the conducting electrons in such a way that there is a complete nonadiabatic process that conserves the spin transfer. It will be shown that the BMR values in atomic size contacts, up to 20 quantum of conductance, have a universal behaviour that is explained as domain wall scattering. Experiments for Ni, Co, Fe, Fe3O4 , CrO2, etc will be shown showing all of them the same type of behaviour.

- **XMCD and thin films?**
  Dimitri Arvanitis

  Uppsala University, Sweden

  I will give an overview on X-ray magnetic circular dichroism of particularly thin films.

- **Theory of XMCD**
  Mike Brooks

  Karlsruhe, Germany

  I will discuss the theoretical background of XMCD.

- **Strategies and future of magnetism at MAX lab**
  Nils Mårtensson

  Uppsala University, Sweden.

  MAX-lab operates two storage rings for synchrotron radiation research. MAX II is a 1.5 GeV third generation machine that provides high brilliance radiation in the soft x-ray regime. Examples of reseach at MAX-lab will be presented. Fifteen beamlines are in operation at MAX-lab. One bending magnet beamline at MAX II

is optimized for magnetic studies using circularly polarized radiation. Furthermore a new insertion device beamline for magnetism research is under construction.

- **Applications of Spin Electronics**
  F. Nguyen Van Dau

  U.M.R. CNRS - Thales, Orsay, France

  I will review our recent development of magnetic devices using several spin dependent transport phenomena.

- **Theory of magnetic semiconductors**
  Susanne Mirbt

  Condensed Matter Theory Group, Uppsala University, Sweden

  I will summarize the current understanding of magnetic semiconductors and dicuss the different existing magnetic coupling models.

- **Experimental results of magnetic properties of thin films**
  Panos Poulopoulos

  Materials Science Department, University of Patras, 26504 Patras, Greece

  The fundamental magnetic observables, i.e. magnetization, Curie temperature, magnetic moment per atom and susceptibility for idealized thin films like Fe, Co, Ni on metal substrates such as Cu, W, Re are measured via conventional laboratory experiments. Surface and interface effects result in strong modifications of the magnetic observables as compared to bulk materials. Magnetic polarization of the 5d elements Pt, Ir and W and the 3d V at the interfaces with the 3d ferromagnets Ni and Fe are probed via the element specific x-ray magnetic circular dichroism. Spin, orbital and total magnetic moments are obtained and trends in the magnetism of the 5d elements are deduced. Monolayer-resolved magnetic moment profiles for the whole multilayer period for Ni and Pt are shown and compared to ab initio calculations.

- **Growth of magnetic semiconducting films**
  Janusz Sadowski

  MAX Laboratory

  The talk presented the details of preparation technique (low temperature molecular beam epitaxy) and reviewed the structural, electrical and magnetic properties of magnetic semiconductor GaMnAs.

- **Growth and characterization of thin films**
  Björgvin. Hjörvarsson

  Uppsala University, Sweden

  I will discuss different experimental techniques allowing to characterize the growth mode of thin films.

- **Industrial aspects of magnetic semiconductors**
  Olle Heinonen

  In this talk, I will explore the potential advantages and technical challenges of semiconductor-based spintronics from the perspective of the magnetic recording industry.

- **Theory of spin dependent transport**
  Nikos Papanikolaou

  Institute of Materials Science, NCSR "Demokritos" GR-15310, Ag. Paraskeui, Athens, Greece

  We presented an overview of the theoretical understanding of spin dependent transport and discussed the giant magnetoresistance effect in metallic multilayers as well as the tunneling magnetoresistance effect in ferromagnet-insulator-ferromagnet junctions. Moreover we described possibilities of spin-injection in ferromagnet-semiconductor junctions in the ballistic regime, and discussed possibilities for spin filtering in metallic nanowires due to defect scattering.

- **Magneto-optics**
  Joachim Schoenes

  The basic theory of magneto-optical spectroscopy is reviewed. It is shown that magneto-optics is a particularly powerful tool to study: spin-orbit splittings in the final state, band splittings in antiferromagnets, empty f-states and j-j coupling.

- **Correlations effects in mesoscopic transport**
  Igor Sandalov

  Condensed Matter Theory Group, Uppsala University, Sweden

  The manifestations of many-body effects in nano-devices are reviewed with particular emphasis on the effects of correlations which influence the spin polarization of the current through such systems.

- **Correlation effects on electronic structure and itinerant-electron magnetism. Dynamical mean-field theory.**
Mikhail I. Katsnelson

Condensed Matter Theory Group, Uppsala University, Sweden.

A review is given of a new approach, LDA+DMFT, to include correlation effects into realistic electronic structure calculations. Applications to finite temperature magnetism of transition metals and to many- body effects in half metallic ferromagnets are considered.

5.1.2 Report on the CECAM/ESF STRUC-Ψ_k Workshop on the Diffusion Quantum Monte Carlo Method

Summary of Workshop

A total of 34 participants from 9 countries attended the workshop held at CECAM from 19 to 21 September 2002. 19 talks and one discussion session covered a wide range of topics from new technical developments to applications of the Diffusion Quantum Monte Carlo (DMC) Method.

The format of the conference gave ample time for discussion, which proved to be extremely useful and productive. The different backgrounds of the participants (mainly physicists and chemists) allowed substantial and fruitful cross-fertilisation. The lively discussions also revealed the high level of activity in the field, which this workshop also served to steer and stimulate.

Brief description of the talks

The first day of the workshop was mainly taken up with talks on variants of the DMC method and on the fixed-node constraint. Michel Caffarel described the possible benefits and drawbacks of the "Pure DMC" method. Cyrus Umrigar described possible algorithms which do not use the fixed-node approximation and possible improvements to the accuracy and efficiency of fixed node algorithms. Mal Kalos described an extension of the DMC algorithm which solves the fermion sign problem, and showed that the new algorithm is stable when dealing with a system of 54 ^{3}He atoms in periodic boundary conditions. Dario Bressanini discussed the form of the nodal surfaces of simple systems, with the goal of developing a way to parameterise the nodes and optimize them directly. Roland Assaraf described new ideas about how to compute observables other than the energy to high accuracy. Heinz-Jürgen Flad proposed a Jastrow factor expressed in a wavelet basis which could be used in DMC calculations and other many-particle methods. The final two talks of the day focussed on applications of the DMC method. Saverio Moroni talked about calculations on ^{4}He droplets aimed at probing superfluid behaviour in confined systems. David Benoit discussed applications to vibrational states of molecules, gaining insight into hydrogen bonding.

The second day of the workshop was concerned with applications of the DMC method, with an emphasis on large systems. Andrew Williamson described highly efficient techniques for dealing with large systems in which the wave functions can be represented by strongly localised orbitals, and presented applications of these methods to semiconductor nanostructures. Ivan Stich presented results for atomic clusters, while Pietro Ballone's talk dealt with the homogeneous jellium system and with jellium clusters. Matthew

Foulkes discussed the problem of calculating the surface energy of jellium, including finite size effects and the small energy differences which must be resolved. Dario Alfè described calculations on the diamond $\Rightarrow$ β-tin phase transition in silicon. The results were not in close agreement with experiment, and a number of possible sources of error were investigated. The day ended with a discussion led by Cyrus Umrigar on the accuracy of DMC calculations. A number of participants presented thoughts and results on time-step errors, pseudopotential errors and finite-size errors. This discussion was very fruitful, exposing problems with present calculations and avenues for further investigation.

The final day of the workshop started with a presentation by Erik Koch of results on lattice models of doped fullerenes. Very interestingly, DMC calculations of the spectral function showed excellent agreement with exact diagonalisation studies. John Trail described mean-field and DMC studies of Wigner crystals. The next three talks concerned the optimisation of trial wave functions. Stephen Fahy described a numerical method for minimising the energy with respect to parameters in the wave function. Peter Nightingale described an elegant generalisation of the standard variance minimisation optimisation procedure which can be applied to excited states. Friedemann Schautz described a method for optimising configuration-interaction coefficients in trial wave functions based on similar ideas to those described in Stephen Fahy's talk. Lubos Mitas presented results for various nanoclusters. In the last talk of the workshop Arne Lüchow presented results for distributed multipole moments and polarisabilities including an analysis of the nodal errors. He also described some ideas on efficient calculations related to those presented earlier in the workshop by Andrew Williamson.

Conclusions

This workshop proved to be a great success. The presentations covered both methodological developments and applications of DMC methods. Stimulating and useful discussions covered most of the areas of interest to the community using these methods.

The popularity of the workshop and the growing number of international groups working in this area suggest that another workshop should be held on this topic within the next few years.

Organisers

Richard Needs, Cavendish Laboratory, University of Cambridge, UK

Claudia Filippi, Universiteit Leiden Instituut-Lorentz for Theoretical Physics, The Netherlands

Mike Towler, Cavendish Laboratory, University of Cambridge, UK

List of Participants

Dario Bressanini	Universita' dell'Insubria, Como, Italy
Saverio Moroni	"La Sapienza", Rome, Italy
Mal Kalos	Lawrence Livermore National Laboratory, Livermore, USA
Stephen Fahy	University of Cork, Cork, Ireland
Arne Lüchow	University of Düsseldorf, Düsseldorf, Germany
Matthew Foulkes	Imperial College, London, UK
Ivan Stich	Slovak Technical University, Bratislava, Slovakia
Michel Caffarel	University of Paris (Jussieu), Paris, France
Roland Assaraf	University of Paris (Jussieu), Paris, France
Lubos Mitas	North Carolina State University, Raleigh, USA
Andrew Williamson	Lawrence Livermore National Laboratory, Livermore, USA
Dario Alfè	University College London, London, UK
Pietro Ballone	University of Messina, Messina, Italy
Cyrus Umrigar	Cornell University, Ithaca, USA
Heinz-Jürgen Flad	MPI für Mathematik in den Naturwissenschaften, Leipzig, Germany
John Trail	University of Cambridge, Cambridge, UK
Erik Koch	MPI für Festkörperforschung, Stuttgart, Germany
Friedemann Schautz	University of Leiden, Leiden, The Netherlands
Peter Nightingale	University of Rhode Island, Kingston, USA
David Benoit	Queen Mary College, London, UK
Claudia Filippi	University of Leiden, Leiden, The Netherlands
Richard Needs	University of Cambridge, Cambridge, UK
Mike Towler	University of Cambridge, Cambridge, UK
Mike Gillan	University College London, London, UK
Maria Alfredsson	Royal Institution, London, UK
Peter Reinhardt	University of Paris (Jussieu), Paris, France
Peter Kratzer	Fritz-Haber Institute, Berlin, Germany
Michele Casula	SISSA, Trieste, Italy
Alexander Badinski	Fritz-Haber Institute, Berlin, Germany
Martin Fuchs	Fritz-Haber Institute, Berlin, Germany
Sami Siljamäki	Helsinki University of Technology, Helsinki, Finland
Neil Drummond	University of Cambridge, Cambridge, UK
Ben Wood	Imperial College, London, UK
Lucas Wagner	North Carolina State University, Raleigh, USA

Programme

Thursday, 19 September		
Chair:	**Claudia Filippi**	
9.30	R.J. Needs	Welcome and Opening Remarks
9.35	M. Caffarel	Stochastic Reconfiguration Monte Carlo: The Best of DMC and Pure DMC
10.20	C.J. Umrigar	Approximate Imaginary Time-evolution Operators With and Without the Fixed-node Approximation
11.00		Coffee
11.30	M. Kalos	Recent Progress in Fermion Monte Carlo
12.15	D. Bressanini	The Nodes of Trial and Exact Wave Functions in Quantum Monte Carlo
13.00		Lunch
14.30	R. Assaraf	Computation of Observables and Small Differences in Energy Using the Zero-variance Property
15.15		Coffee
15.30	H.-J. Flad	Merging Quantum Monte Carlo with Conventional Many-Particle Methods
16.15	S. Moroni	Quantum solvation of Carbonyl Sulfide with Helium atoms
17.00	D. Benoit	Vibrational Orbitals: A New Perspective on Hydrogen Bonding
17.45		Close

Friday, 20 September		
Chair:	**Mike Towler**	
9.30	A.J. Williamson	Quantum Monte Carlo Simulations of Semiconductor Nanostructures
10.15	I. Stich	QMC study of Electronic Correlation in Cluster Systems
11.00		Coffee
11.30	P. Ballone	QMC Computations for Homogeneous and Inhomogeneous Jellium Systems
12.15	W.M.C. Foulkes	Quantum Monte Carlo Studies of Jellium Surfaces
13.00		Lunch
14.30	D. Alfe	The Diamond $\Rightarrow$ β-tin Transition in Silicon from Diffusion Monte Carlo Calculations
15.15		Coffee
15.30	C.J. Umrigar	Discussion of Accuracy of DMC Calculations
17.00		Close

Saturday, 21 September		
Chair:	**Richard Needs**	
9.30	E. Koch	Fixed-node Monte Carlo for Fermions on a Lattice: Applications to the Doped Fullerenes
10.15	J. Trail	QMC Studies of 2D and 3D Wigner Crystals
11.00		Coffee
11.30	S. Fahy	Energy Optimization of Variational Wave Functions in Solids: General Theory and Calculation of the van der Waals Energy in Graphite
12.15	P. Nightingale	Optimization of Trial Wave functions for Excited States of Bosonic Clusters
13.00		Lunch
14.30	F. Schautz	Optimization of CI Coefficients in Multi-determinant Jastrow-Slater Wave Functions
15.15		Coffee
15.30	L. Mitas	Electronic Structure of Nanosystems and Solids by Quantum Monte Carlo Methods
16.15	A. Lüchow	Distributed Multipole Moments and Polarizabilities with DMC
17.00		Close

Abstracts

Stochastic Reconfiguration Monte Carlo: The Best of DMC and Pure DMC

Michel Caffarel[1], Roland Assaraf[1], and Anatole Khelif[2]

[1] *CNRS-Lab. de Chimie Théorique, Tour 22-23, Case Courrier 137, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cedex 05, France*

[2] *CNRS-Lab. de Logique Mathimatique, Universite Denis Diderot, 2 place Jussieu, 75251 Paris Cedex 05, France*

Among the several variants of quantum Monte Carlo approaches the most popular one is certainly the Diffusion Monte Carlo (DMC) method. It is based on a combination of a drifted diffusion process and a birth/death (or branching) process. In practical calculations, these two processes are realized by applying some simple stochastic rules to each member of a finite population of "walkers". Because of the branching term the number of walkers is not constant and a population control step is required. Unfortunately, this additional step introduces a finite error. For large enough number of walkers and for accurate enough trial wave functions this error can be made negligible. However, when trial wave functions are poor or when no trial wave function is used (e.g., in vibrational studies of floppy molecules), this is no longer true. In addition, computation of dynamical

quantities are not properly defined in a presence of a branching term. A simple remedy to these various problems is to remove the birth/death step and to introduce the branching weight into the averages (to "carry" the weights). In principle, this method -known as the Pure diffusion Monte Carlo method (PDMC)- is quite attractive: In contrast with DMC the number of walkers is fixed, there is no bias due to the population control, the error made for a finite simulation time is under control, and the various correlation functions in time can be defined without difficulty. Unfortunately, in practice the method is unstable and works only when accurate trial wave functions are used (weights close to one). In this talk we present a method based on the use of a so-called stochastic reconfiguration step instead of branching [1,2]. Our motivation is to combine the best of both worlds: efficiency of DMC and absence of bias as in PDMC. The approach is derived within a PDMC framework (the walkers "carry" some weight) but the population is reconfigured using some specific rules. These rules are chosen so as to minimize as much as possible the statistical fluctuations and also to recover the PDMC and DMC methods as two well-defined limits.

1. R. Assaraf, M. Caffarel, and A. Khelif, Phys. Rev. E **61**, 4566 (2000).
2. M. Caffarel, R. Assaraf in Mathematical models and methods for *ab initio* Quantum Chemistry in Lecture Notes in Chemistry, eds. M. Defranceschi and C. Le Bris, Springer p.45 (2000).

Approximate Imaginary Time-evolution Operators With and Without the Fixed-node Approximation

Cyrus J. Umrigar

Cornell Theory Center, Cornell University, Ithaca, NY 14853, USA

I will define some measures of the error in time-evolution operators, that I think are of relevance to DMC and apply these to the errors in some approximate importance sampled real-space representations of the time-evolution operator, both with and without imposing fixed-node boundary conditions. One goal is to construct a "cross-node" algorithm, similar to Ceperley's release-node algorithm, that employs a Fermionic guiding function in contrast to Ceperley's bosonic guiding function. This could be combined with Sorella's stochastic reconfiguration ideas could be used to control the growth of the non-fermionic components of the distribution of walkers.

Recent Progress in Fermion Monte Carlo

M. H. Kalos

Lawrence Livermore National Laboratory Livermore, CA 94551, USA

We have been studying an extension of Diffusion Monte Carlo that solves the "sign problem" of fermions. The modifications to standard DMC comprise: (a) Random walkers carry signs. That is, their contributions to estimators of projected integrals required for an energy quotient are given algebraic signs. (b) Distinct guiding functions are used for walkers of different signs. (c) The Gaussians that determine diffusion for pairs of opposite walkers are correlated in such a way that the walkers drift towards each other. (d) Opposite walkers in a pair cancel when close.

Is can be shown that if the results are stable– that is, if the denominator of the energy quotient does not decay at large imaginary times, the the results are correct for fermionic systems. Experimentally, the method has been shown to be stable for periodic systems of He^3 atoms, and for small systems of electrons. We will describe the method in more detail, and give the computational results for some first-row dimers.

The Nodes of Trial and Exact Wave Functions in Quantum Monte Carlo

Dario Bressanini

Dipartimento di Scienze Chimiche, Fisiche e Matematiche Universit' dell-Insubria Via Lucini 3, 22100 Como, Italy

Although quantum Monte Carlo is, in principal, an exact method for solving the Schrödinger equation, systems of Fermions still pose a challenge. Thus far all solutions to the "sign problem" remain inefficient (or wrong). The fixed-node approach, however, is efficient, and in many situations remains the best approach. If only we could find the exact nodes, or at least a systematic way to improve the nodes, we would, in effect, bypass the sign problem.

Despite the fundamental importance of quantum wave functions, very little is known about their nodal structure. A detailed knowledge of the topology of these high-dimensional surfaces is a necessary step for improvement of trial nodes and a systematic study has never been attempted, despite the obvious consequences for improving quantum simulations that such knowledge might generate. Such improvement would be of great benefit to quantum simulations, which could then be systematically improved within the context of the fixed-node approximation. Here we review what is known about nodes, show some recent results on simple atomic and molecular systems, and formulate some conjectures. A long term goal of this research is to develop a way to directly parametrize the nodes of accurate trial wave functions and optimize them directly.

Computation of Observables and Small Differences in Energy Using the Zero-variance Property

Roland Assaraf and Michel Caffarel

Laboratoire de Chimie Théorique, CNRS et Université Paris VI, Case Courrier 137, 4, place Jussieu, 75252 Paris Cedex 05, France

Over the recent years quantum Monte Carlo (QMC) methods have become more and more successful in computing ground-state total energies of molecular systems. For a variety of systems including organic molecules, clusters of atoms, solids etc... the accuracy obtained by QMC is impressive. In most cases, the quality of the results is comparable or superior to that obtained with traditional techniques: DFT, MCSCF or coupled cluster (CC) methods. Unfortunately, the calculation with QMC of properties other than energy turns out to be much more difficult.

In this talk we present some recent progress toward computing efficiently observables. It is shown how the zero-variance principle responsible for the high-level of accuracy on total energies can be applied to other properties. In analogy with energy calculations, the lower the variance of some "renormalized" expression of the observable is, the more accurate the expectation value is. As a consequence, observables can be computed with a high accuracy at the variational level. As an important application we show how forces between atoms (gradient of the energy with respect to nuclear coordinates) can be calculated using our formalism. Finally, we discuss how this scheme can be extended to compute accurate small differences of energy.

Merging Quantum Monte Carlo with Conventional Many-Particle Methods

Heinz-Jürgen Flad

Max-Planck-Institut für Mathematik in den Naturwissenschaften
Inselstr. 22-26, D-04103 Leipzig, Germany

The success of quantum Monte Carlo (QMC) methods is intimately linked to the availability of accurate trial wavefunctions. Due to the requirement of QMC for a compact representation of the trial wavefunction, only limited use has been made so far from the large variety of wavefunctions provided by other many-particle methods in quantum chemistry. On the other hand it is also difficult to transfer insight gained from QMC on the structure of the wavefunction into these methods.

We propose a Jastrow type ansatz for the wavefunction based on methods from multi-scale analysis, which might help to bridge the gap. Herein the Jastrow factor is approximated in a wavelet basis, which enables a local and adaptive representation, especially in the cusp regions. Due to the tensor product structure of the many-particle wavelet basis it is possible to apply standard methods from quantum chemistry, like coupled electron pair approximations, to specify the variational parameters of the expansion. The resulting matrix elements can be expressed in terms of one- and two-electron integrals avoiding exceedingly complicated higher dimensional integrals. These wavefunctions can be used as trial wavefunctions in diffusion Monte Carlo calculations, providing an improved flexibility for the description of electron correlations. Vice versa it is possible to expand parts of

a Jastrow factor, already successfully applied in QMC calculations, in the wavelet basis and use it within other many-particle methods in order to achieve a reduction of the variational degrees of freedom and an improved convergence behaviour.

Quantum solvation of Carbonyl Sulfide with Helium atoms

Saverio Moroni
"La Sapienza", Rome, Italy

Rotational spectroscopy of molecules embedded in ^{4}He nanodroplets offers a unique tool for probing superfluid behaviour in confined systems. The theoretical understanding of superfluidity in doped Helium clusters presently relies on permutation cycles in finite-temperature path integral simulations, hydrodynamical models, or limited knowledge of excited states. We introduce a novel ground-state estimator for the effective moment of inertia of the molecule and relate its dependence on the number of Helium atoms to current-current correlations and density profiles. The moment of inertia features a maximum for about ten Helium atoms, and for larger clusters quickly reaches its asymptotic value. Results are compared with recent measurements for He_N-OCS clusters.

Vibrational Orbitals: A New Perspective on Hydrogen Bonding

David M. Benoit
Department of Chemistry, Queen Mary College, University of London, Mile End Road, London E1 4NS, UK

Vibrational delocalisation of weakly bound complexes amongst minima of similar potential energy is of great importance in spectroscopy. This quantum effect has a bearing on the shape of clusters, such as hydrogen-bonded complexes, making their rotational spectra difficult to analyse. Unfortunately, a harmonic treatment fails to give an accurate description of the vibrational ground state needed to elucidate these spectra and a high-quality method is needed to rationalise the observations. We show that nuclear diffusion Monte Carlo (RB-DMC) is an efficient and robust technique to treat such problems, readily providing ground-state-averaged properties. Moreover, its combination with a powerful wave-function analysis tool, based on one-body density representation, gives insights into the nature of hydrogen bonding in clusters of biological interest.

Quantum Monte Carlo Simulations of Semiconductor Nanostructures

Andrew Williamson, Randy Hood, Jeff Grossman, Aaron Puzder and Giulia Galli
Lawrence Livermore National Laboratory, USA

A method for performing QMC calculations where the computational time required to evaluate the local energy of a configuration of electron coordinates scales linearly with the

number of electrons will be presented. Truncated, maximally localized Wannier functions are chosen to represent the single particle orbitals in the Slater determinant part of the many-body wavefunction. This choice or orbitals yields increasingly sparse Slater determinants as the system size is increased. As the evaluation of the Slater determinant and its derivatives is typically the most time intensive part of a QMC calculation, the ability to use sparse operations yields a near linear scaling of the computational time required to evaluate the total energy of a single configuration of electron coordinates. Recent advances to this approach using non-orthogonal Wannier functions will be presented.

The application of these QMC techniques to the evaluation of a variety of optical properties of silicon quantum dots will be presented. The benchmark level of accuracy that can be achieved within the fixed node, diffusion quantum Monte Carlo approach enables QMC calculations to be used as a tool for evaluating the accuracy of more conventional electronic structure techniques. We present a comparison of the size dependence of optical gaps predicted by QMC, density functional and semi-empirical techniques. We also present results of a study of the effects of structural relaxations of the excited state geometry of silicon quantum dots, the Stokes shift, to predict the energy difference between optical absorption and emission in quantum dots.

QMC Study of Electronic Correlation in Cluster Systems

P. Bokes[1], I. Stich[1], and L. Mitas[2]

[1] *Center for Computational Materials Science (CCMS), Dept. of Physics, Slovak Technical University (FEI STU), Bratislava, Slovakia*

[2] *Dept. of Physics, North Carolina State University, Raleigh, U.S.A.*

We use a number of electronic structure methods, including DFT, post-SCF, and QMC to study a range of cluster systems (ionic hydrogen clusters, silicon clusters), surfaces in cluster model (Si(001)), and biological molecules (porphyrines). It is shown that the correlation energy is responsible for ordering of the different potential energy minima in these systems and that the energy differences in ordering may be surprisingly large. The importance of a proper treatment of electronic correlation will be demonstrated on systems where mean-field treatment leads to a total failure of the system description. In the opposite limit, we will discuss on the example of the Si(001) surface whether a correlated method can discern unequivocally an energy difference between two structures (buckled or symmetric dimers on the Si(001) surface) separated in energy by $\approx$0.1 eV. These systems will serve to highlight the strengths and limitation

QMC Computations for Homogeneous and Inhomogeneous Jellium Systems

Pietro Ballone

University of Messina, Italy

Jellium systems provide a suitable playground to check the predictions of many-body theories by QMC computations. I present Fixed-Node Diffusion MC results for homogeneous and inhomogeneous systems.

In the case of homogeneous systems, the focus is on the paramagnetic to ferromagnetic transition and on the Wigner crystallization. I present new results, and I discuss the comparison with previous computations.

In the case of inhomogeneous systems, I present results for isolated and for interacting jellium spheres. In the case of isolated spheres, total energy, electron and spin density have bee computed for a wide range of sizes and background densities. The QMC results are compared to the predictions of recent approximations for the exchange and correlation energy proposed by J.P. Perdew and co-workers. Interacting jellium spheres provide benchmark results for non-local correlations in valence electron systems.

Quantum Monte Carlo Studies of Jellium Surfaces

B. Wood[1] and W.M.C. Foulkes[1], and Mike Towler[2]
[1] *Imperial College of Science, Technology and Medicine, UK*
[2] *University of Cambridge, UK*

Recently, Yan *et al.* [1] cast doubt on the accuracy of all existing Quantum Monte Carlo studies of jellium surfaces. One possible source of inaccuracy in previous calculations may be an insufficiently detailed treatment of the finite-size errors related to the Coulomb interaction. We have been studying jellium slabs using a different implementation of this interaction, and present the preliminary results of our investigations here.

1. Z. Yan, J. P. Perdew, S. Kurth, C. Fiolhais, and L. Almeida, Phys. Rev. B 61, 2595 (2000).

The Diamond $\Rightarrow$ β-tin Transition in Silicon from Diffusion Monte Carlo Calculations

Dario Alfè[1], Mike Gillan[1], Mike Towler[2], and Richard Needs[2]
[1] *University College London, UK*
[2] *University of Cambridge, UK*

The first principles determination of the phase transition properties of materials has been traditionally tackled using density functional theory (DFT) techniques. Absolute errors in DFT energy calculations can be of the order of one eV/atom, which is far too large. However, the great success obtained in a large number of problems relies on cancellation of

errors between different phases. Nevertheless, in some cases this cancellation is not sufficient. The diamond$\rightarrow$ β-tin transition in silicon is one example in which DFT calculations based on the Local Density Approximation (LDA) wrongly predict the transition pressure, with an error of about 40 %. A similar scenario is the calculation of the zero pressure melting temperature of silicon, which is underestimated by about 20 % within DFT-LDA. Both these erroneous predictions arise from a non-cancellation of the DFT-LDA errors in the two phases. Quantum Monte Carlo (QMC) based calculations are expected to deliver much greater precision, with absolute errors in calculated energies possibly not larger than a tenth of one eV/atom. However, the intrinsic complexity of QMC calculations has traditionally restricted its range of applications. Here we present some preliminary results for the diamond $\Rightarrow$ β-tin transition in silicon using Diffusion Monte Carlo (DMC) techniques, with non-local pseudopotentials and the fixed node approximation. Early indications show that DMC over-corrects the DFT-LDA result, possibly overestimating the transition pressure by as much as 40 %.

Discussion of Accuracy of DMC Calculations

Discussion Led by Cyrus J. Umrigar
Cornell Theory Center, Cornell University, Ithaca, NY 14853, USA

The most important sources of errors in diffusion Monte Carlo (other than the obvious statistical error) are probably:

1. **Time-step error and fixed-node error**. See my talk.

2. **Population control error**. It is well known that it is inversely proportional to the size of the target population. In practice it is frequently, but not always, negligible compared to other errors. The error can be estimated using the method of Nightingale and Blote and of Hetherington (also described in my 1993 paper with Nightingale and Runge) even when it is much smaller than the statistical error. This is useful when one is forced to use a small target population.

3. **Pseudopotential error**. What is the justification for using DFT or HF pseudopotentials in QMC? Claudia Filippi, and, Richard Needs and coworkers have independent evidence that HF pseudopotentials work better in QMC than LDA ones. The Cambridge group is building a library of HF pseudopotentials for use in QMC. How convincing is the evidence? Is there any advantage to using OPM/OEP pseudopotentials instead of HF? Could one add some approximate correlation to either HF or OEP to further improve? What are the prospects for more fundamentally correct approaches, such as that in the Acioli-Ceperley paper, or the semiempirical construction of Lee-Kent-Towler-Needs-Rajagopal? Acioli-Ceperley did not do anything beyond Li. LKTNR had good results for Si at least. Does it help to use core-polarization potentials?

4. **Pseudopotential locality error in DMC**. Most people just seem to assume that this is small, but what is the evidence for that? I have tested the locality error for the Si_2 dimer by using the same single determinant in conjunction with a sequence of seven progressively better Jastrow functions. The difference in the energy obtained from the 0^{th}-order Jastrow (no Jastrow) and the 6^{th}-order Jastrow is 14 mH, which is certainly not negligible. Claudia had, prior to me, observed a 13 mH difference between the energies obtained with an e-e Jastrow and an e-e-n Jastrow, using a different pseudopotential. What is the experience of other researchers?

5. **Finite size errors**. This error can be considerable for periodic systems. The CASINO code developed by the Needs group implements the Model Periodic Coulomb (MPC) interaction (in addition to the standard Ewald interaction) which reduces the Coulomb component of this error. Ceperley's group has developed the twist-averaged boundary condition method. How well do these work?

Jeff Grossman in a very recent JCP has performed a systematic study of the accuracy of DMC. He calculated the atomization energies of 55 molecules. He finds that the mean absolute deviation from experiment is 2.9 kcal/mol and the largest deviation is 13 kcal/mol and discusses the likely causes of these errors. What would it take to do much better than this?

People who would like to contribute to the discussion should come prepared, if possible, with a couple of viewgraphs. It would he helpful, but not necessary, for me to know before hand who would like to contribute.

Fixed-node Monte Carlo for Fermions on a Lattice: Applications to the Doped Fullerenes

Erik Koch
Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Fullerides are crystals made from C_{60}-molecules. Doping these crystals with electrons puts charge carriers into the band derived from the lowest unoccupied molecular orbital of C_{60}, doping with holes adds carriers to the band derived from the highest unoccupied level. Since the Coulomb repulsion between charges on the same C_{60}-molecule is strong, it is essential to include correlation effects for understanding the behavior of the induced charges. We show how the correlated hopping of the induced carriers between the C_{60}-molecules can be described using a multi-band Hubbard model. Such a lattice model can be treated using the fixed-node approximation adapted for lattice models. We demonstrate the importance of choosing appropriate trial functions and describe efficient ways for optimizing their parameters. As applications we discuss results for the Mott transition as a function of orbital degeneracy and dimensionality of the system. In addition we show calculations of response-functions that help understanding the metallic and superconducting properties of the doped Fullerenes.

QMC Studies of 2D and 3D Wigner Crystals

J. R. Trail, M. D. Towler, N. D. Drummond and R. J. Needs
TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, UK

We have developed new trial wave functions for 2D and 3D Wigner crystals based on a mean-field approach. These wave functions give new insights into the physics of the crystalline state and provide an excellent starting point for QMC calculations. This approach leads to improved accuracy and efficiency of VMC and DMC studies of Wigner crystals. Our scheme should allow the development of better trial wave functions for more complicated systems such as defective Wigner crystals and Wigner molecules.

Energy Optimization of Variational Wave Functions in Solids: General Theory and Calculation of the van der Waals Energy in Graphite

Stephen Fahy
University of Cork, Ireland

We will review recently developed variational Monte Carlo methods for the minimization of energy with respect to the parameters in a general class of Jastrow-Slater wave functions that are suitable for periodic solids. We will demonstrate their use in explicitly calculating the contribution of van der Waals correlation to the interlayer binding of graphite, as follows: Using a modified many-body Hamiltonian, long-range instantaneous electron interactions are replaced by a static Hartree potential, thereby eliminating van der Waals correlations. This produces an optimal groundstate trial wave function which, in combination with the true fully-interacting Hamiltonian, determines the energy of the system when long-range correlation is removed.

This talk is based on work over a number of years with David Prendergast, Claudia Filippi, Friedemann Schautz, David Bevan, Antonella Malatesta, and Giovanni Bachelet. We acknowledge support from Enterprise Ireland, The Irish Higher Education Authority, and Science Foundation Ireland.

Optimization of Trial Wave Functions for Excited States of Bosonic Clusters

Peter Nightingale
Department of Physics, University of Rhode Island, Kingston, Rhode Island, USA

I shall discuss progress in the optimization of excited state trial wavefunctions,[1,2] in addition to applications of this method, using correlation function Monte Carlo approach, of ground and excited state energies of bosonic van der Waals clusters. The calculations are performed employing trial wavefunctions with general four-body correlations.

1. M. P. Nightingale and Vilen Melik-Alaverdian, "Optimization of ground and excited state wavefunctions and van der Waals clusters", Phys. Rev. Lett. 87, 43401 (2001).

2. M. P. Nightingale and Vilen Melik-Alaverdian, "Trial function optimization for excited states of van der Waals clusters", in "Recent Advances in Quantum Monte Carlo Methods - Part II", edited by William A. Lester, Jr., Stuart M. Rothstein and Shigenori Tanaka, World Scientific (Singapore 2002), p. 127.

Optimization of CI Coefficients in Multi-determinant Jastrow-Slater Wave Functions

Friedemann Schautz
Instituut-Lorentz for Theoretical Physics, Universiteit Leiden, The Netherlands

A quantum Monte Carlo method for obtaining multi-determinant Jastrow-Slater wave functions for which the energy is stationary with respect to variations of CI coefficients is presented. The single particle orbitals can also be optimized simultaneously. Using ground state calculations of atoms and small molecules as illustrative examples, the method is shown to converge rapidly and to significantly lower the energy in most cases. Additionally, we discuss preliminary results obtained using this optimized multi-determinant trial wave functions for the ground state and low excited states within fixed-node diffusion Monte Carlo.

This work was done in collaboration with Stephen Fahy (University College Cork, Ireland) and Claudia Filippi (Universiteit Leiden, The Netherlands)

Electronic Structure of Nanosystems and Solids by Quantum Monte Carlo Methods

Lubos Mitas, P. Sen, L. K. Wagner, Z. Helms
Department of Physics, North Carolina State University, USA

We report on our recent Quantum Monte Carlo calculations of the electronic structure for several types of nanosystems and solids such as Si nanoclusters with embedded transition metal atoms, molecules involving transition metal atoms and transition metal oxide solids. We focus on calculations of ground and excited states in order to elucidate the electronic gaps and some optical properties. Several approaches were tried such as combination of diffusion Monte Carlo and Configuration Interaction, correlated sampling and direct state-by-state calculations. This enabled us to identify the ground states in TM@Si_x nanoclusters with competing d-states localized on the TM atom and more extended states from p-orbitals of the Si skeleton. We also attempt to predict band gaps of solid materials for which the experimental results are contradictory or inconclusive.

Distributed Multipole Moments and Polarizabilities with DMC

Arne Lüchow
University of Dusseldorf, Germany

Distributed Multipoles can be calculated routinely with standard ab initio methods. They provide an important ab initio tool for the construction of intermolecular potentials. Since multipole moments are sensitive to correlation effects, they are a good candidates for property calculation with DMC. It is shown how distributed multipole moments and polarizabilities can be calculated easily with DMC. The effect of the node location error on the results is analysed.

5.1.3 Report on the XII Workshop on Computational Materials Science

23 to 29 September 2002
Villasimius (Cagliari), Sardinia, Italy

The twelfth edition of the Workshop on Computational Materials Science [formerly known as Computational Condensed Matter (1990-1994) Italian-Swiss (1990-1997) Workshop] was held on the south-eastern coast of Sardinia, Italy from 23 to 29 September. The main sponsors were the *High Level Scientific Conferences* Program of the European Community (HPCF-CT-2000-00322) and the Ψ_k European Science Foundation Program; UNESCO bestowed its prestigious patronage. Nearly 90 participants gathered at the Workshop, in the pleasant framework of the Sofitel Timi Ama sea resort, in an informal atmosphere also favored by excellent weather. As customary in this workshop, social and scientific programs blended together nicely (a two-evening poster session was the highlight) favoring intense discussion and contacts.

The traditional focus of this workshop is ab initio electronic structure, mostly within density-functional theory. Tight binding and ab initio molecular dynamics, as well as less-common topics such as polarization theory have been well represented in past editions. While keeping with the tradition of past meetings, this workshop has devoted some attention to semiempirical and model approaches, to statistical mechanics, biophysics, biological modelling, and experiment. This implies (given the sum rule on the workshop length) that the cross section of each single topic is somewhat smaller than usual, but this program formula had the definite merit of opening up new perspectives and contacts in the form of new or unfamiliar viewpoints, besides the obviously necessary confrontation with inputs from experiment. A somewhat arbitrary classification of the 18 one-hour invited talks shows that there were 9 ab initio ones, 2 on statistical mechanics-related topics, 1 on semiempirical, classical, and analytical methods, 4 on biophysics and biological modelling, and 2 on experiments.

One of the ab initio studies focused on DFT basics, such as DFT beyond the adiabatic approximation and current density-functional theory (Rubio), while the talks of Jonsson and Zunger were devoted to reviews on fundamental problems in semiconductor physics that can be tackled with appropriate combinations of first principles calculations and methods derived from statistical mechanics. A second talk of Zunger revisited the familiar concept of the doping under a new point of view. Jonsson gave a second lecture on the strategy to bridge time scales during simulations of relevant processes, as the ones occurring during epitaxial growth. Eichler presented DFT calculations on aspects related to adsorption and reaction on metal surfaces and on zirconia surfaces. Zirconia has been the subject of Fiorentini's talk where the possible use of zirconia (and hafnia) as gate oxides for Si electronics has been discussed on the basis of DFT calculations. These High-K oxides have

been studied by Först with the Projector Augmented Wave Method within the framework of DFT calculations. The two theoretical talks on these oxides were introduced by the exciting experimental talk by Fanciulli who illustrated application to nanoelectronics and spintronics. Semiempirical methods and large scale simulations were called into play by Colombo in his talk on triple junction in polycristalline silicon, while Jensen presented results on growth of metal clusters on metal surfaces. A exciting overview on quantum annealing was due to Santoro who explained the method and its applications to complex systems. Finally, the biophysics section reviewed two *extremes* of the theoretical research in the fields: on one side, results on molecular motors obtained with coarse grained models were presented by Lattanzi, on the other side, accurate QM/MM simulations on drugs and membrane channels (Carloni) provided remarkable insights into the microscopic mechanisms governing fundamental biological processes and drug action. This section was completed by the experimental talk of Gratton who described spectroscopy methods to investigate fluctuations in biological membranes.

Contributed talks (10) gave to young scientists the opportunity of presenting their results on new methods, on surface physics, on electron-density response, on molecular switch. The range of topics mirrored the spectrum of the invited talks. The over 50 posters presented in two lively evening sessions focused mostly on ab initio (with some semiempirical tight binding blend) simulations. Among the topics touched upon, let us mention ab initio study of aromatic hydrocarbons in astrophysically relevant conditions, metal and semiconductor surface dynamics, lattice dynamics of semiconductors, quantum structures, electronic structure of nanowires, electronic properties of quantum dots, transport in network of quantum dots, optical properties, nanostructures etc.

The available abstracts of the lectures, of the contributed talks and the list of posters follows below.

INVITED TALKS

Structure and function of membrane channels from computer simulation

Paolo Carloni

SISSA, via Beirut 4, 34014 Trieste (Italy)

Abstract not available

Ab initio approach to proteins of pharmaceutical relevance

Paolo Carloni

SISSA, via Beirut 4, 34014 Trieste (Italy)

Abstract not available

Triple junctions in polycrystalline silicon

Luciano Colombo

INFM and Dept. Physics, Univ. Cagliari (Italy)

Polycrystalline silicon (poly-Si) displays a complex arrangment of grain boundaries (GBs) joining at triple junctions (TJs). Any topological modification of the poly-Si microstructure should be therefore described as a competing interaction among GBs and TJs. Nevertheless, it is usually attributed to GBs motion only, the TJs role being solely limited to preserve the proper angle between GBs at the thermodynamical equilibrium. At variance with the above scenario, we proved by atomistic simulations that a TJ in poly-Si is in fact a true defect (characterized by a positive line energy and a measurable volume contraction), acting as a stress concentrator. By means of constant-traction molecular dynamics investigations, we adrress two problems: (i) the three-sided grain annihilation process at a multiple-twin TJ; and (ii) its response to external load. In particular, we investigate either an ideal and an indented junction, establishing the TJ elastic stability limit and the propagation features of a crack tip moving towards the core of the line junction. This work has been supported by INFM-MUSIC and MIUR-PRIN2000 projects.

Adsorption and reaction of small molecules on metal surfaces

Andreas Eichler

Institut für Materialphysik and Center for Computational Materials Science, Universität Wien

Density functional theory can contribute a lot to the understanding of microscopic processes going on during adsorption and reaction at surfaces. However, in most cases the more interesting quantities are at a macrocopic level, as there are sticking coefficients, reaction rates or phase diagramms. In this talk a few possibilities will be presented of how to extend this microscopic description into the macroscopic world. The first part of the talk is devoted to the description and exploration of potential energy surfaces (PES) of molecules over surfaces. At the example of oxygen over Pt(111) it will be shown how - on the basis of the DFT-PES [1] - macroscopic quantities like sticking coefficient can be obtained, by employing tight binding molecular dynamics [2]. In the second part of the talk CO oxidation reactions (CO+NO,CO+O) [3,4] will be discussed. Apart from activation energies and reaction pathways also reaction rates are presented by combining harmonic transition state theory with DFT results.

Structure of (Y-doped) zirconia surfaces and adsorption of Pt

Andreas Eichler

Institut für Materialphysik and Center for Computational Materials Science, Universität Wien

In the last few years zirconia has experienced much attention in industry: as support material in catalysis, for metal coatings and as ion conductor in gas sensors. In this study the structure and ion conductivity of tetragonal Y-stabilized zirconia is studied in the

bulk phase [1]. Based on the optimized bulk structure an investigation of the surface of pure and Y-doped zirconia is presented. Interestingly, dependent on the surface termination an enrichment (111-surface) or reduction (001-surface) of Y-defects at the surface is predicted. For the very similar cubic modification a surface phase diagram as a function of oxygen and hydrogen chemical potentials is presented. Finally potential energy surfaces for the adsorption of Pt on the surface of pure and Y-doped zirconia are discussed.

High-k dielectrics for nanoelectronics and spintronics

Marco Fanciulli

Laboratorio MDM - INFM, Via C. Olivetti 2, 20041 Agrate (MI), Italy

Abstract not available

Evaluation of zirconia and hafnia as gate oxides for Si electronics

Vincenzo Fiorentini and **Gianluca Gulleri**

INFM and Dept. Physics, Univ. Cagliari (Italy)

Parameters determining the performance of the crystalline oxides zirconia (ZrO_2) and hafnia (HfO_2) as gate insulators in nanometric Si electronics are estimated via ab initio calculations of the energetics, dielectric properties, and band alignment of bulk and thin-film oxides on Si (001). With their large dielectric constants, stable and low-formation-energy interfaces, large valence offsets, and reasonable (though not optimal) conduction offsets (electron injection barriers), zirconia and hafnia appear to have a considerable potential as gate oxides for Si electronics.

Introduction to the Projector Augmented Wave Method and Applications Related to High-K Gate Oxides

Clemens J. Först,[(1,2)] **Christopher Ashman**,[(1)] **Karlheinz Schwarz**,[(2)] and **Peter E. Blöchl**[(1)]

[(1)] *Institute of Theoretical Physics, Clausthal University of Technology, Leibnitzstraße 10, 38678 Clausthal-Zellerfeld, Germany*

[(2)] *Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, 1060 Vienna, Austria*

Scaling of semiconductor devices currently results in structures with nearly atomic dimensions. Gate oxides, which separate the switching current from the drive current in a MOSFET transistor, are approaching a thickness range of only few atomic layers, so that quantum-mechanical leakage currents become intolerable. New insulating materials with larger dielectric constants, e.g. high-k oxides, can be implemented at a larger physical thickness with electrical properties equivalent to those of an ultrathin conventional gate oxide.

We give a short introduction to the projector augmented wave method and show its application in the context of ab-inito molecular dynamics simulations on early transition

metal (Zr, Hf) adsorption on Si(001). We investigated the total energy surface for an isolated adatom and continually increased the coverage up to two monolayers. The simulations indicate that a spontaneous silicide formation takes place. These results are in agreement with a number of experimental results reported so far and improve the global understanding of processes during oxide growth at the atomic level.

Growing controlled nanocluster films

Pablo Jensen

Département de Physique des Matériaux, UMR CNRS 5586, Université Claude Bernard Lyon-1, 69622 Villeurbanne Cédex, FRANCE

I will present recent results on the growth of nanostructured films prepared by cluster deposition. After the surprisingly high values for cluster diffusivity found on graphite surfaces, we investigated cluster diffusion on a variety of different substrates, to understand technologically important experimental issues. The simulation results are compared to experiments.

Long time scale simulations of metal crystal growth: The importance of multi-atom processes

Hannes Jonsson

Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

Abstract not available

Self-diffusion and dopant atom clustering in silicon: Successes and failures of DFT

Hannes Jonsson

Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

Abstract not available

Application of coarse grained models to the analysis of macromolecular structures

Gianluca Lattanzi

Hahn-Meitner Institut, Glienickerstrasse 100, 14609 Berlin (Germany)

We review some of the computational methods that have been recently applied to the study of biological macromolecules, i.e. DNA, RNA, carbohydrates and proteins. The latter ones, in particular, have been the subject of intense studies aimed at understanding not only their equilibrium properties, but also their dynamics. However, in most cases of biological importance, the size of these molecules and the time scale on which they operate prevent from a direct application of all atoms techniques and demand the development of

computationally efficient, yet physically sound, coarse grained models. We examine some recent advances in this field, and describe the Gaussian and Anisotropic Network Model, that have been recently applied to a variety of different proteins and nucleic acids. We finally show some preliminary results on the application of coarse grained models to the kinesin monomer and dimer.

Coarse grained models: the kinetics of motor proteins

Gianluca Lattanzi

Hahn-Meitner Institut, Glienickerstrasse 100, 14609 Berlin (Germany)

Motor proteins are able to transform the chemical energy of ATP hydrolysis into mechanical work that is essential for a variety of tasks in living cells. Major advances in single molecule nanomanipulation have made it possible to measure the displacements of these proteins along linear tracks, and therefore to obtain an approximate description of their kinetics. Discrete and continuous stochastic models are particularly suited to the interpretation of experimental data in this field, since both allow a complicated mechanochemical process to be coarse grained in relatively few parameters. However both of them present advantages and shortcomings, though usually one model succeeds where the other fails. We have recently developed a coarse graining procedure, based on a renormalization group scheme, that accounts for the force dependence of transition rates in discrete models, bridging a gap between the two stochastic approaches. We discuss the main results obtained with this procedure and possible future directions of investigation.

Quantum annealing of complex systems

Giuseppe Santoro

SISSA, Trieste

Abstract not available

The Inverse band structure approach : given a property, find the structure

Alex Zunger

National Renewable Energy Laboratory, Golden CO 80401, USA

Abstract not available

Fundamental limits of doping in semiconductors

Alex Zunger

National Renewable Energy Laboratory, Golden CO 80401, USA

Abstract not available

CONTRIBUTED TALKS AND POSTERS

Improved classical force field for hydrogen bonding, J. Akola, P. Ballone, R.O. Jones

Institut für Festkörperforschung, Forschungszentrum Jülich.

Calculations of twist boundaries in strontium titanate, R. Astala and P. D. Bristowe

Department of Materials Science and Metallurgy, University of Cambridge, UK

A first principles investigation of mercuric iodide: bulk properties and intrinsic defects, F. Ayres, L. V. C. Assali, W. V. M. Machado, J. F. Justo

Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil

MD simulations of a [2]Catenane-based molecular switch , Matteo Ceccarelli, F. Mercuri, D. Passerone, and M. Parrinello

Swiss Center for Scientific Computing, 6928 Manno, Switzerland

Misfit dislocations at a highly mismatched semiconductor interface, Giancarlo Cicero, Laurent Pizzagalli*, and Alessandra Catellani

INFM and Physics Department, Polytechnic of Torino, * University of Poitiers, France

Understanding Ferroelectricity in H-bonded materials by ab initio calculations the case of KH2PO4(KDP) and KD2PO4(DKDP), G. Colizzi,[1] J. Kohanoff,[1] S. Koval,[2] and R. Migoni[2]

[1] The Queen's University of Belfast (UK)

[2] Universidad Nacional de Rosario (Argentina)

Ab initio calculation of the infrared absorption spectrum of Germanium and Silicon, G. Deinzer and D. Strauch

Institut für theoretische Physik, Universiät Regensburg, D-93040 Regensburg, Germany

Emerging magnetism in ultrathin 4d and 5d transition metal nanowires , Anna Delin[1] and Erio Tosatti[1,2,3]

[1]ICTP, Strada Costiera 11, 34100 Trieste, Italy

[2]SISSA, via Beirut 4, 34014 Trieste, Italy

[3]INFM, Trieste, Italy

Energetics and diffusion of B in Ge and SiGe, Pietro Delugas and Vincenzo Fiorentini

INFM and Dept. Physics, Univ. Cagliari (Italy)

Origin of the efficient light emission for inversion domain boundaries in GaN, Vincenzo Fiorentini

INFM and Dept. Physics, Univ. Cagliari (Italy) **Effects of the crystal structure in the dynamical electron-density response of hcp transition metals**, I. G. Gurtubay,[1] Wei Ku,[2], J. M. Pitarke,[1,3], and A. G. Eguiluz[4,5]

[1] Materia Kondentsatuaren Fisika Saila, Euskal Herriko Unibertsitatea, 644 P.K, 48080 Bilbo, Basque Country, Spain

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Donostia, Basque Country, Spain
[4] Department of Physics and Astronomy, Univ. of Tennessee, Knoxville, TN 37996-1200, USA
[5] Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-1200, USA

Ab initio calculations of superconducting properties via Density-Functional Theory , A. Floris,[1] S. Massidda,[1] G. Profeta,[2] A. Continenza,[2] M. A. L. Marques,[3] M. Lüders,[4] N. N. Lathiotakis,[5] L. Fast,[5] and E.K.U. Gross[5]
[1] Dipartimento di Fisica, Università di Cagliari, I-09042 Monserrato (CA), Italy
[2] Dipartimento di Fisica, Università di L'Aquila, I-67010 Coppito (AQ), Italy
[3] Departamento de Física de Materiales, Facultad de Químicas, Universidad del País Vasco; Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC), San Sebastián, Spain
[4] Condensed Matter Theory, SISSA, Trieste, Italy

[5] Fachbereich Physik, Freie Universität Berlin, Germany

Structural, electronic and magnetic properties of the complex perovskite $PbFe_{1/2}Ta_{1/2}O_3$, Cesare Franchini, Nathascia Lampis, Guido Satta, Sandro Massidda, Alessandra Geddo Lehmann
INFM-Dipartimento di Fisica, Università di Cagliari

Ab-initio **study of the Imma phase in Silicon**, Katalin Gaál-Nagy and Dieter Strauch
Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg

Site preference for CO adsorption on close-packed transition metal surfaces from DFT, Marek Gajdoš, Andreas Eichler, and Jürgen Hafner
Institut für Materialphysik and Center for Computational Materials Science

The role of prismatic dislocation loops in the generation of glide dislocations in Cz-silicon, A. Giannattasio, S. Senkader, R. J. Falster,* P. R. Wilshaw
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GaP(001) Hydrogen terminated surface structures from first principles , P. H. Hahn,[1] O. Pulci,[1] R. Del Sole,[1] W. G. Schmidt,[2] and F. Bechstedt[2]
[1]Tor Vergata University, Rome, Italy
[2]Computational Materials Science Group, University of Jena, Germany

An ab initio investigation on the structural and eletronic properties of Ti impurities in SiC , K. O. Barbosa, L. V. C. Assali, W. V. M. Machado, and J. F. Justo
Universidade de São Paulo, São Paulo, Brazil

Modeling dislocations in silicon and in gallium arsenide with ab initio methods , J. F. Justo, L. V. C. Assali, R. W. Nunes
Escola Politécnica, Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil

Nickel impurities in diamond: a first principles investigation , R. Larico, L. V. C. Assali, W. V. M. Machado, and J. F. Justo
Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil

Influence of Electron-Electron Interactions on Supercurrent in SNS structures, Klas E. Engström, Jari Kinaret, Robert Shekhter, Martti Puska,[§] and Henri Saarikoski[§]
Department of Applied Physics, Chalmers University of Technology and Göteborg University, Sweden
[§]Laboratory of Physics, Helsinki University of Technology, Finland

Oxygen on Pd(111): The formation of a surface oxide, C. Klein, G. Kresse, E. Lundgren, M. Borg, J.N. Andersen, M. De Santis, Y. Gauthier, C. Konvicka, M. Schmid and P. Varga
Institut für Allgemeine Physik, Vienna University of Technology, A-1040 Vienna, Austria

Three-body self-interstitials and the W line in Si, Giorgia Lopez and Vincenzo Fiorentini
INFM and Dept. Physics, Univ. Cagliari (Italy)

Coulomb couplings in positively charged fullerenes, Martin Lüders,[1,2] Andrea Bordoni,[3] Nicola Manini,[1,3,4] Andrea Dal Corso,[1,2] Michele Fabrizio,[1,2,5] and Erio Tosatti[1,2,5]
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Nonlinear finite element calculations of residual stress in dislocated crystals, Paweł Dłużewski and Grzegorz Maciejewski
Institute of Fundamental Technological Research, Świętokrzyska 21, 00-049 Warsaw

Predicting crystal structures: Parrinello-Rahman method revisited, Roman Martoňák, Alessandro Laio, and Michele Parrinello
Swiss Center for Scientific Computing, Via Cantonale, CH-6928 Manno, Switzerland *and* ETH Zurich, Physical Chemistry, Hoenggerberg, CH-8093 Zurich, Switzerland

Long-range contribution to the xc-kernel of TDDFT, Valerio Olevano,[1] Silvana Botti,[1] Francesco Sottile,[1] Nathalie Vast,[1] Lucia Reining,[1] Angel Rubio,[2] and Giovanni Onida[3]
[1] Laboratoire des Solides Irradiés, CNRS-CEA, École Polytechnique, F–91128 Palaiseau, France
[2] Departamento de Física de Materiales, Facultad de Ciencias Químicas, Universidad del Pais Vasco, and Donostia International Physics Center. E–20018 San Sebastián, Basque Country, Spain
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Tight-Binding Approach for the Solution of hopping transport in Random

Networks of Quantum Dots, Marta Prada and P. Harrison
School of Electronic and Electrical Engineering, University of Leeds, LS2 9JT, UK

Ab initio study of the Sb-induced 1x1 reconstruction on Si(001), Olivia Pulci
INFM, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy

Wigner molecules in polygonal quantum dots: A density functional study, Esa Räsänen, Henri Saarikoski, Martti Puska, Risto Nieminen
Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, 02015 HUT, Finland

Combined quantum and classical methods to map electric field onto nanostructured carbon aggregates, Walter Rocchia,[1] Laura Zoppi,[2] and Luciano Colombo[2]
[1] Research Centre "E. Piaggio" – University of Pisa Via Diotisalvi, 2 - 56126 Pisa - Italy
[2] Department of Physics, University of Cagliari, Cittadella Universitaria I-09042 Monserrato (CA) (Italy)

Ab intio study of CO Adsorption on a NiO(100) surface using the LDA+U method, Adrian Rohrbach, Georg Kresse, and Jürgen Hafner
Institut für Materialphysik and Center for Computational Material Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

Transport and chaotic scattering in LSSL heterojunctions, Giovanni Santoboni and Franco Meloni
INFM-Dipartimento di Fisica, Università di Cagliari

Rotational profiles of electronic absorption bands of polycyclic aromatic hydrocarbons in astrophysically relevant conditions: ab initio approach, G. Malloci, G. Mulas, G. Cappellini, G. Satta and P. Benvenuti
Dipartimento di Fisica, Università di Cagliari, Cagliari (Italy)

Ab-initio Optical Properties of BN(110) and GaN(110) Surfaces, Guido Satta,* Giancarlo Cappellini,* Maurizia Palummo, ** and Giovanni Onida***
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∗ ∗ ∗ INFM – Dipartimento di Fisica, Università di Milano, I-20133, Milano, Italy

Electronic structure of Ag-Pd heterostructures, Matthieu Verstraete, Jacques Dumont,* Robert Sporken,* and Xavier Gonze
PCPM Unit, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
* LISE Facultés universitaires Notre Dame de la Paix, Naumr, Belgium

Grand Canonical Monte Carlo Simulations of Hydrogen in Carbon Nanostructures, Manuela Volpe,[1,2] Laura Zoppi,[3] Fabrizio Cleri,[1] and Luciano Colombo[3]
[1] ENEA, Centro Ricerche Casaccia, Divisione Materiali, CP 2400, I-00100 Roma (Italy)
[2] Department of Chemical Science and Technology, University of Roma Tor Vergata, Rome, Italy

[3] Department of Physics, University of Cagliari, Cittadella Universitaria I-09042 Monserrato (CA), Italy

Multiplet structure of fullerene ions, Małgorzata Wierzbowska, Martin Lüders, and Erio Tosatti
The Abdus Salam International Centre for Theoretical Physics

Deformation potentials of tetrahedral semiconductors from linear-response theory, Rinaldo Zucca,[a,b] Pasquale Pavone,[b] and Vincenzo Fiorentini[a]
[a]) INFM and Dipartimento di Fisica, Universitá di Cagliari, Italy
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5.1.4 Report on CECAM–ESF/Ψ_k Workshop

AB INITIO THEORETICAL APPROACHES TO THE ELECTRONIC STRUCTURE AND OPTICAL SPECTRA OF MATERIALS

CECAM, Lyon, France
23–25 September 2002

Organisers:
Pablo García-González (Universidad Autónoma de Madrid, Spain)
Maurizia Palummo (Università di Roma "Tor Vergata", Italy)
Olivia Pulci (Università di Roma "Tor Vergata", Italy)
Arno Schindlmayr (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)
Nathalie Vast (Ecole Polytechnique, Palaiseau, France)

The CECAM–ESF/Ψ_k Workshop "Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials" was held in Lyon during 23–25 September 2002 with the aims of assessing the present status of ab initio approaches for the spectroscopic properties of finite and infinite systems, establishing links between scientists from different communities working on excited states, and developing and promoting new solutions. In total, 58 scientists from ten European countries as well as the United States and Japan attended the meeting.

The principal focus of the workshop was recent developments in Green-function approaches and time-dependent density-functional theory. In both fields, sophisticated approximations and advances in the computational techniques now allow accurate quantitative calculations and applications to increasingly complex systems. Examples that were presented at the workshop included excitons on semiconductor surfaces and in nanocrystals as well as the quasiparticle electronic structure of surface defects. Methodical developments, especially for the calculation of dielectric functions and total energies, formed the second main topic. Different ways of including vertex corrections were discussed on the basis of model calculations and asymptotic properties that allow a critical assessment. The programme was completed by talks about excitations in strongly correlated systems and transport, which made connections to neighbouring fields.

The workshop programme consisted of 13 invited and 12 contributed talks. Twenty further contributions were presented in a poster session. In line with the workshop's aims, much time was devoted to discussions, not only after each talk, but also during a plenary round-table discussion. This exchange of opinions was seen as particularly beneficial and inspired a number of follow-up investigations.

The programme is included below together with the abstracts of invited and contributed talks. The poster abstracts as well as further information about the event is available at

http://www.fisfun.uned.es/∼athaesos/

The workshop was generously sponsored by the ESF Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (STRUC–Ψ_k), the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and the Commissariat à l'Energie Atomique (C.E.A.).

PROGRAMME

Monday, 23 September 2002

Total Energies

9:00 Opening and announcements

9:15 **Rex W. Godby**
Total energies from self-energy operators

9:50 **Nils-Erik Dahlen**
Variational many-body functionals for the total energy of atoms

10:10 **Bengt Holm**
Pair correlation functions from GW calculations

10:30 Coffee

Total energies/Exchange and correlation

11:00 **Xavier Gonze**
Density functionals based on the adiabatic-connection fluctuation-dissipation formula: Application to H_2 and Be_2

11:35 **Yann-Michel Niquet**
Exchange-correlation potentials in the adiabatic-connection fluctuation-dissipation theorem

11:55 **Arno Schindlmayr**
Density-functional approach for the electronic self-energy

12:15 **Patrick Rinke**
Exchange and correlation effects in small jellium clusters

12:35 Lunch

Excitations in strongly correlated systems

14:30 **Marie-Bernadette Lepetit**
Ab initio calculation of local excited states in strongly correlated systems

15:05 **Charles H. Patterson**
Ab initio exchange coupling-constant calculations for manganites and cuprates

15:40 Discussion

16:00 Coffee

Posters

16:30 Short oral presentations

17:00 Poster session

Tuesday, 24 September 2002

Excitons

9:00 **Michel Mareschal** (Director of CECAM)
Welcome address

9:10 **Brice Arnaud**
Electron-hole excitations in semiconductor and insulators

9:45 **Michael Rohlfing**
Surface excitons at insulator interfaces

10:05 **Friedhem Bechstedt**
Excitons in confined systems: Surfaces and nanocrystals

10:40 Coffee

Excitons/Polarisation functions

11:00 **Andrea Marini**
Dynamical excitons in metals and semiconductors

11:20 **Eric Shirley**
Aspects of polarizabilities in real materials:
Models and symmetry properties

11:55 **Stefan Kurt**
Time-dependent optimized effective potential: An approach to the vertex

12:30 Lunch

Exchange-correlation kernels

14:30 **Valerio Olevano**
Long-range contribution to the exchange-correlation kernel
in time-dependent density-functional theory

14:50 **Rodolfo Del Sole**
Long-range behaviour and frequency dependence of
exchange-correlation kernels in semiconductors

15:25 **Oleg Pankratov**
Many-body diagrammatic expansion for the exchange-correlation
kernel in time-dependent density-functional theory

16:00 Coffee

Transport and dynamics

16:30 **Barbara Tobiyaszewska**
Current throug finite 1D wires: Non-equilibrium Green's function approach

16:50 **Peter Bokes**
Self-consistent current-carrying steady states
from a maximum-entropy principle

17:10 Round-table discussion

Core-level and defect spectra

9:00 **Carl-Olof Almbladh**
Effects of core-level degeneracy and crystal fields on core-level spectra

9:35 **Stefano de Gironcoli**
Temperature effects on surface core-level shifts

10:10 **Magnus Hedström**
Quasiparticle band structure of the As vacancy on GaAs(110)

10:30 Coffee

Dielectric response

11:00 **Silvana Botti**
Ab initio calculations of the anisotropic dielectric tensor of GaAs/AlAs superlattices

11:35 **Apostolos Marinopoulos**
Ab initio calculations of the dielectric response of graphite and small-diameter carbon nanotubes

12:00 Closing remarks

12:30 Lunch

ABSTRACTS OF INVITED AND CONTRIBUTED TALKS

Total energies from self-energy operators

R. W. Godby[1], P. García-González[2], K. T. Delaney[1], P. Rinke[1], and T. Gould[1]

[1] *Department of Physics, University of York, United Kingdom*

[2] *Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain*

Progress has become slow in constructing ever better approximations to the exact Kohn-Sham energy functional of density-functional theory that are applicable in a wide range of situations, reflecting the extreme complexity of the exact functional, including its *ultra-non-local* dependence on the electron density in certain situations. These non-analyticities in the exchange–correlation energy functional may be circumvented by reformulating the total energy using Green's-function many-body perturbation theory, as a practical alternative to DFT. A real-space-imaginary-time representation offers an efficient framework for implementing a fully self-consistent GW approximation, which is a conserving approximation. We show results for total energies of homogeneous and inhomogeneous systems within GW [1]. We also discuss prospects for improved density-based models of self-energies. Building on earlier work [2], these would allow inexpensive total-energy calculations within the framework of a generalised Kohn-Sham theory.

[1] P. García-González and R. W. Godby, Phys. Rev. Lett. **88**, 056406 (2002).

[2] P. Sánchez-Friera and R. W. Godby, Phys. Rev. Lett. **85**, 5611 (2000).

The application of variational many-body functionals to the total energies of

atoms

N.-E. Dahlen and U. von Barth

Solid State Theory Group, Physics Department, Lund University, Sweden

In the present work we have tested variational energy functionals obtained from many-body perturbation theory in a number of atoms. We have tested the functional due to Luttinger and Ward (LW) as well as the recently proposed functional due to Almbladh, von Barth and van Leeuwen (ABL). The functionals are variational in the sense that they can be evaluated at rather crude approximations to their independent variables which are (i) the one-electron Green function, and (ii) the Green function and the screened interaction respectively for the two functionals mentioned. The quality of the results will depend on the level of sophistication of the underlying perturbation expansions. The functionals were previously applied to the electron gas and shown to be extraordinarily accurate already at the level of the so called GW approximation (GWA). At the same level, they have also been applied to linear Hubbard chains with less encouraging results. We here find that the LW functional, at the GW level, corrects approximately half the error in the RPA correlation energies of atoms. In going to second order in the screened interaction we find it important to make full use of the variational property of the ABL functional with respect to the screened interaction. Evaluation of the latter functional at a non-interaction Green function and a statically screened interaction gives errors in the correlation energies of atoms of the order of 10–20%.

The actual calculations are of a complexity that would allow for these methods to be applied also to molecules and solids. Our applications to molecular binding energies are in progress.

Pair correlation functions from GW calculations

Bengt Holm[1] and Ulf von Barth[2]

[1]*Dept. of Physics, Graduate School of Science, University of Tokyo, Japan*

[2]*Solid State Theory Group, Physics Department, Lund University, Sweden*

The GW method is emerging as one of the leading tools to calculate excited states in a many body system. In the formulation of the theory, a self consistent procedure is prescribed. However, since self consistency is time consuming and makes calculations complicated, the usual implementations of the GW approximation involve what is usually referred to as a one iteration scheme.

In the presentation, some light will be shed on the properties of self consistency. Further, results of the calculation of total energies are presented, and we discuss the properties of pair correlation functions generated from various Green's functions; the ones from self-consistent, partially self-consistent and one iteration schemes respectively.

Density functionals based on the adiabatic-connection fluctuation-dissipation theorem: Application to H_2 and Be_2

X. Gonze[1], M. Fuchs[1,2], Y.-M. Niquet[1], K. Burke[3]
[1] *Universite Catholique de Louvain, Belgium*
[2] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*
[3] *Rutgers University, USA*

Fully nonlocal exchange-correlation functionals derived from the adiabatic-connection fluctuation-dissipation theorem can go beyond local or gradient corrected functionals and include the van der Waals interaction. We implement three functionals of this class, in a pseudopotential plane-wave framework, (1) using the random-phase approximation (RPA), (2) adding to the RPA short-range correlations (RPA+), and (3) beyond RPA, including an approximate exchange kernel. We work in a non-self-consistent framework, starting from the converged exact-exchange (only for H_2) or LDA Kohn-Sham potential. We find the binding energy of the H_2 and Be_2 molecules described, by all three functionals, within 0.1 eV accuracy. Equilibrium bond lengths and harmonic vibrational frequencies generally improve upon LDA and GGA. We then explore the H_2 full dissociation curve. The ACFD approach solves the "DFT symmetry-dilemma" encountered for large H_2 internuclear separations, but creates an unphysical potential barrier to dissociation, for distances on the order of 5 bohrs.

Exchange-correlation potentials in the adiabatic-connection fluctuation-dissipation framework

Y.-M. Niquet[1], X. Gonze[1], and M. Fuchs[1,2]
[1] *Unité PCPM, Université Catholique de Louvain, Belgium*
[2] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

We investigate the possibility of making self-consistent calculations of the total energy in the adiabatic connexion fluctuation dissipation (ACFD) framework. We provide the ACFD exchange-correlation (xc) potential in the general case, and focus on the random-phase approximation (RPA) as an example. We establish the links between the ACFD-RPA and the many-body perturbation theory in the *GW* approximation, both at the level of total energy (Luttinger-Ward formula) and xc potential (Sham-Schlüter equation). We show that the ACFD-RPA xc potential is likely to diverge far from a finite system, due to the presence of the empty kohn-sham states in the expression of the ACFD-RPA total energy. We discuss the implications of this divergence for self-consistent ACFD calculations, and propose some modified potentials that exhibit correct asymptotic behaviour.

Density-functional approach for the electronic self-energy

Arno Schindlmayr
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Within density-functional theory a perturbation series that yields the exact quasiparticle excitation energies in terms of the Kohn-Sham orbitals and eigenvalues in derived. In

contrast to a coupling-constant expansion of the self-energy, the present scheme is designed such that the first-order term includes dynamic screening and closely resembles the non-self-consistent GW approximation, which is widely used in electronic-structure calculations. However, it also solves some known deficiencies of the latter. In particular, it is internally consistent, the spectral function integrates to the correct particle number in every order of perturbation theory, and the energy of the highest occupied state always equals the exact chemical potential. The perturbation series provides a systematic procedure for generating higher-order self-energy corrections beyond the GW approximation.

Exchange and correlation effects in small jellium clusters

P. Rinke[1], P. García-González[2], and R. W. Godby[1]

[1] *Department of Physics, University of York, United Kingdom*

[2] *Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain*

We present *ab initio* electronic structure calculations for small, spherical jellium clusters or quantum dots (QD) in the GW self-energy approach. In particular we analyse the effects of exchange and correlation, which give rise to image effects in these structures.

In recent years, GW (G: Green function, W: screened Coulomb potential) has successfully been applied to calculate band structures of bulk materials and surfaces as well as properties of small molecules and clusters. We apply *ab initio* many-body perturbation theory (MBPT) in the GW approximation to solve the quasiparticle equation, using a space-time approach [1] for the self-energy.

We analyse the structure of the self-energy operator in real-space including its non-locality and frequency dependence. Substantial changes (up to about 1 eV) in the quasiparticle energy spectrum are observed, which arise in part from physical effects inherently absent in other methods such as density-functional theory (DFT), in the usual approximations. The wave functions for unoccupied states near the vacuum level deviate considerably from eigenstates of the DFT system at similar energy, which we attribute mainly to image effects at the surface of the cluster. A comparison with calculations based on a classical electrostatic image potential [2] is made.

[1] H. N. Rojas, R. W. Godby and R. J. Needs, Phys. Rev. Lett. **74**, 1827 (1995)

[2] P. Rinke, MSc Dissertation: *Image Effects in Quantum Dots* (1999)

Ab initio calculation of local excited states in strongly correlated systems

Marie-Bernadette Lepetit

Université Paul Sabatier, Toulouse, France

The physics of strongly correlated materials have attracted a lot of attention in the last two decades. These systems are strongly multiconfigurational in nature and the ab-initio methods such as DFT usually fail to decribe their low energy physics and fascinating properties. There physics is usually described by model Hamiltonians with local effective interactions that can be extracted from the low energy local spectroscopy. The present

talk will show the key ingredients necessary for the determination of accurate local excitations. We will discuss in particular the importance of the crystal environment, of the multiconfigurational nature of the wave-function of the dynamical polarisation and correlation effects.

Ab initio exchange coupling-constant calculations for manganites and cuprates

Charles H. Patterson, G. Zhengg, and M. Nicastro

Department of Physics, Trinity College, Dublin, Ireland

Strongly correlated electron materials are generally studied using model Hamiltonians with parameter values adjusted to give best fits to experiment. We present results of bulk Unrestricted Hartree-Fock (UHF) and cluster configuration interaction (CI) calculations on $LaMnO_3$, $La_{0.5}Ca_{0.5}MnO_3$ and La_2CuO_4, from which exchange coupling constants and low-lying excitation energies are extracted. Cluster CI calculations are performed in a localised orbital basis and configurations in the ground state wave function show which quantum fluctuations are important in determining exchange coupling energies. A localised orbital basis also permits an easy mapping to a model Hamiltonian. Calculations of the exchange coupling constants in $LaMnO_3$ show good agreement with experimentally derived values; UHF calculations on $La_{0.5}Ca_{0.5}MnO_3$ show that the ground state contains only d^4 Mn ions and both O^{2-} and O^- ions. Hence a double-exchange Hamiltonian is inappropriate for doped manganites. Cluster CI calculations of the exchange coupling constants in La_2CuO_4 show reasonable agreement with experimentally derived values.

Electron-hole excitations in semiconductors and insulators

Brice Arnaud[1], Sebastien Lebegue[2], and Mebarek Alouani[2]

[1] *GMCM, Campus de Beaulieu, Rennes, France*

[2] *IPCMS, Strasbourg, France*

Ab initio calculations of the electronic structure of insulators entail big difficulties involved with the treatment of excitation energies and many-body effects. The most successful first-principles method, the density functional theory (DFT) within the local density approximation (LDA) is designed for ground state properties and can not provide a proper description of the band structures of insulators. However, it is possible to accurately calculate the quasiparticle energies and band gaps from first principles by solving Hedin's set of equations for the full Green's function in the so-called GW approximation.

An approach based on an *all-electron* method (PAW) has been developed to compute the quasiparticle energies within the GW approximation. Within this approximation, the self-energy is given as a product of the one-particle Green's function G and the dynamically screened interaction W computed within the random phase approximation (RPA). Starting from the calculated local density approximation (LDA) ground state, the LDA eigenvalues are corrected by treating the difference between the self-energy and the exchange-correlation potential as a perturbation. The calculated quasiparticle energies

obtained by means of this procedure are, generally, in good agreement with photoemission experiments, and are found to be neither sensitive to the scheme used for decoupling core and valence electrons nor to the different plasmon-pole models used to reproduce the frequency dependence of the dynamically screened interaction W.

The quasiparticle spectra are then used to compute the imaginary part of the macroscopic dielectric function including both local-field and excitonic (electron-hole attraction) effects. The standard procedure for including these effects in the calculation of the dielectric function consists in solving the so called Bethe-Salpeter equation. This approach has been applied to different semiconductors and insulators, and it has been shown that the inclusion of electron-hole attraction is crucial for an adequate comparison of the theoretical and experimental optical spectra.

Surface excitons at insulator surfaces

M. Rohlfing, N.-P. Wang, P. Krüger, and J. Pollmann

Institut für Festkörpertheorie, Universität Münster, Germany

We investigate the properties of excited electronic states at insulator surfaces from first principles. Based on density functional theory for the electronic ground state, single-particle excitations and coupled electron-hole excitations are discussed within many-body perturbation theory (GW approach and Bethe-Salpeter equation). The electron self-energy operator and the corresponding electron-hole interaction kernel are treated within the GW approximation. As one prototype example, we discuss surface excitons at the LiF(001)-(1×1) surface, that lead to a characteristic surface peak in the reflectivity spectrum of the material. Work on clean and adsorbate-covered MgO surfaces is under progress.

Excitons in confined systems: Surfaces and nanocrystals

Friedhelm Bechstedt

Friedrich-Schiller-Universität, Jena, Germany

Ab initio calculations of optical spectra and pair excitation energies are presented for nanostructures such as semiconductor surfaces and nanocrystals including the interaction of electrons and holes. Two different approaches are used. For calculations of spectra usually the polarization function has to be computed by solving the Bethe-Salpeter equation. We replace it by the solution of an initial-value problem for the time-dependent polarization. As examples reflectance-anisotropy spectra of semiconductor surfaces are calculated. In order to calculate pair excitation energies a special ΔSCF method is used. The total energy of the excited system with electron-hole pair is calculated under an occupation constraint for the HOMO state of the ground-state system. The method is applied to Ge, Si, and $Ge_{1-x}Si_x$ nanocrystals. Pair excitation energies are obtained for singlet and triplet excitons versus diameter and composition. Stokes shifts are discussed.

Dynamical excitons in metals and semiconductors

A. Marini[1] and R. Del Sole[2]

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[2]*Istituto Nazionale per la Fisica della Materia–Dipartimento di Fisica dell'Università di Roma "Tor Vergata", Italy*

It is well known that to reproduce correctly the experimental absorption spectrum of semiconductors both self–energy and excitonic effects are required. However only quasi-particle corrections are usually included while the dynamical renormalization factors $Z_{\rm qp}$ are not. When included, the renormalization of the single–particle spectral functions strongly reduces the spectral intensity worsening considerably the theoretical absorption spectrum if compared with the experimental results. Using a generalized ladder approximation we show that the solution of the Bethe-Salpeter equation in the presence of a frequency dependent screened interaction $W(\omega)$ can be rewritten in terms of a new effective two particle kernel $\Pi(\omega)$. This kernel is itself an expansion in terms of the screened interaction but we show that only terms up to the second order in $W(\omega)$ are important. We show that the presence of a frequency dependent potential $\Pi(\omega)$ renormalizes the non–interacting electron–hole Green's function and the static electron–hole interaction compensating dynamical self–energy effects and reproducing the well–known excitonic effects observed experimentally.

It is also well known that metals do not seem to exhibit any *static* excitonic-like effect. However in the present scheme *dynamical* excitonic effects in metals are possible and indeed occur, as we show in the case of copper. The absorption spectrum turns out to be in agreement with experimental results when both self–energy and excitonic effects are included.

Aspects of polarizabilities in real materials: Models and symmetry properties

Eric L. Shirley

NIST, US Department of Commerce, Gaithersburg, USA

The community continually makes great progress in ab initio and model polarizabilities for real materials. Polarizabilities are ubiquitous in condensed matter. This talk will address two practical examples: the macroscopic optical properties of wide-gap insulators used in photolithography, and calculations of the screened potential of a core hole in a solid. Optical properties are described by the dielectric tensor relating electric field and displacement. In cubic systems, this tensor is isotropic, except for effects of finite wavelength of light. The effects of finite wavelength might have a significant effect on transmissive optical elements in the deep ultraviolet. Here, related symmetry-breaking effects are calculated. This symmetry breaking gives insight into anisotropies of excitons, including energies and oscillator strengths. In the Bethe-Salpeter calculations, great care was taken to suppress spurious symmetry-breaking effects. Calculating the screening of a core hole or other charged defect in a solid can depend on detailed calculation of the two-point irreducible (RPA) polarizability. Here, we shall present development and results of

model calculations that attempt to calculate the polarizability more efficiently. Aspects of sum-rules and scaling properties will be touched on.

Time-dependent optimized effective potential: An approach to the vertex

Stefan Kurth[1] and Ulf von Barth[2]

[1] *Institute for Theoretical Physics, Free University Berlin, Germany*

[2] *Solid State Theory Group, Department of Physics, Lund University, Sweden*

The proper description of optical absorption has been a long-standing problem within many-body perturbation theory. It is well known that in the GW approximation, the dressing up of the one-electron Green function results in optical absorption intensities which are much too low. In addition, the essential f-sum rule for the linear density response function is no longer satisfied, unless the particle-hole interactions or vertex corrections are properly accounted for. The main problem is thus to dress up Green functions and simultaneously include particle-hole interactions in a dynamically consistent way. One possibility is to use time-dependent Hartree-Fock (TDHF) theory , but this has so far proven to be too complicated to apply, even for simple systems as the uniform electron gas.

Time-dependent density functional theory (TDDFT) provides an alternative description of optical absorption. While the popular adiabatic local density approximation (ALDA) gives reasonable absorption spectra for atoms, it is inadequate for insulators. Here we study the next level of approximation beyond the ALDA, the optimized effective potential (OEP). In the exact exchange version of static DFT (or exchange-only OEP), the nonlocal Hartree-Fock potential is replaced by the local, exact exchange potential. Similarly, the integral equation for the response function of TDHF is here replaced by an explicit expression for the exact exchange kernel of TDDFT. The scheme is consistent in the sense that it results in a response function which obeys the f-sum rule at the same time as it provides a dynamic vertex with proper analyticity. We present encouraging results for atoms and the uniform electron gas and argue that applications to molecules and solids are within reach.

Long range behavior and frequency dependence of exchange-correlation kernels in solids

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We define an effective exchange-correlation kernel $f_{xc}^{\rm eff}$ which allows to obtain correct absorption and energy loss spectra starting from an electronic structure obtained within some given approximation. We consider, in particular, the Kohn-Sham electronic structure calculated in the Local-Density Approximation, and the one obtained from a quasiparticle calculation. We show that in both cases, the main feature able to account for

the experimental spectra is a sizeable, complex, frequency and material dependent long-range contribution to $f_{xc}^{\rm eff}$. We write, in terms of this contribution, an expression for the macroscopic dielectric function which is a generalization of the well-known contact-exciton approximation. For silicon and diamond, accurate absorption and electron energy loss spectra are obtained.

We also outline a method to calculate the xc kernel without solving the Bethe-Salpeter equation. Application to bulk Si yields an excellent optical spectrum at a reduced computational cost. The method looks promising for treating complex systems.

Long-range contribution to the xc-kernel of TDDFT

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Starting from the many-body Bethe-Salpeter equation we derive [L. Reining et al., Phys. Rev. Lett. **88**, 066404 (2002)] an exchange-correlation kernel f_{xc} that reproduces excitonic effects in bulk materials within time-dependent density functional theory. The resulting f_{xc} accounts for both self-energy corrections and the electron-hole interaction. It is *static*, *non-local* and has a long-range Coulomb tail. Taking the example of bulk silicon and other semiconductors as well as insulators, we show that the $-\alpha/q^2$ divergency is crucial and can, in the case of continuum excitons, even be sufficient for reproducing the excitonic effects and yielding excellent agreement between the calculated and the experimental absorption spectrum. We also show that, within the range of validity of the method, the parameter α depends linearly on the inverse of the dielectric constant.

Many-body diagrammatic expansion for the exchange-correlation kernel in time-dependent density-functional theory

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Time-dependent density-functional theory (TDDFT) is a promising method for the calculation of excitation energies of many-electron systems. However, the analytical properties of the dynamic exchange-correlation (xc) kernel f_{xc}, which plays a key role in TDDFT (similar to XC-potential in DFT), are largely unknown. We developed the diagrammatic rules for a perturbative expansion of f_{xc} using the Kohn-Sham-based many-body diagrammatic technique. In this technique the Kohn-Sham (KS) Green's functions are the basic propagators and the diagrammatic representation of the xc-potential arises from the requirement that the KS density is exact. We find that at KS frequencies $f_{xc}(\omega_{ij})$ is infinitely-ranged (in extended systems), which is closely related to the discontinuity of the xc-potential. We also show that $f_{xc}(\omega_{ij})$ has no singularities at KS transition energies ω_{ij}

in every order of the perturbation theory. However, it may diverge with the system size if the states $|i\rangle$ and $|j\rangle$ are delocalized. This signifies that any particular perturbative approximation for f_{xc} requires a consistent perturbative treatment of the response function (that is, it should be treated in the same order, but not in any "better" approximation!) to avoid uncontrollable errors in the many-body corrections to the excitations energies.

Current through finite 1D wires: Non-equilibrium Green's functions approach

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We study the charge transport phenomena in 1D atomic wire in nonlinear regime. To model this system we use finite chain connected to macroscopic leads (which play the role of reservoirs). All parts (chain and leads) are described by tight-binding Hamiltonian. In the chain we include additionally the on-site and inter-site interactions which establish proper shape of potential along the chain. The formula for current is obtained from Keldysh non-equilibrium Green's functions (NEG) and the nonlinear I-V curves have been calculated. The influence of system parameters (i.e. coupling between leads and chain, chain length and interactions) on transport has been analyzed.

Self-consistent current-carrying steady states from a maximum entropy principle

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We suggest that a reasonable approach to describe current-carrying steady states at the *ab-initio* level in nanostructures could be built on general grounds of the maximum entropy principle for the statistical density matrix [1]. The presence of an imposed electrical current is reflected as a non-equilibrium constraint on the maximization of the information entropy. The requirement of time-independence of the ensemble introduces another Lagrange multiplier, the λ operator. While the λ operator complicates the calculation significantly for an interacting system, we develop a generalised density-current functional scheme and discuss the simplest nontrivial functional that can be used. We relate our approach to other maximum entropy calculations [2], and compare the method to the widely employed occupation scheme for current-carrying calculations [3].

[1] E. T. Jaynes, in *The Maximum Entropy Formalism*, edited by R. D. Levine and M. Tribus (MIT Press, Cambridge, 1978), pp. 15–118.

[2] See e.g. O. Heinonen and M. D. Johnson, Phys. Rev. Lett. **71**, 1447 (1993).

[3] A. McCann and J. S. Brown, Surf. Sci. **194**, 44 (1988).

Effects of core-level degeneracies and crystal fields on core-level spectra

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Effects of core-level degeneracies on x-ray photoemission spectra (XPS) are considered theoretically and computationally. Processes within each degenerate sub-level manifold are treated by a leading-order cumulant approximation, and processes which connect spin-orbit or crystal-field split levels to leading order in the core-electron self energy. The cumulant approximation is consistent with earlier asymptotic results and correctly describe the leading moments of the core-electron spectrum. The central quantity in both cases is an exponent function which may be expressed in terms of projected state densities and core-valence Coulomb matrix elements. In the past, only the core-valence exchange interaction has been taken into account, but in the general case also the direct core-valence interaction couples the core sublevels. Numerical results are presented for the Al $L_{2,3}$ and the Rh and Pd $M_{4,5}$ levels and compared with recent experiments. In the case of Rh $M_{4,5}$, the level-dependent effects are strong leading to an increased asymmetry, a much increased lifetime width of the M_4 level, and deviation from Lorentzian lifetime broadening. In Pd, the effects are much weaker owing to a much smaller d density of states at the core-hole atom, and it is almost negligible in Al, the most noticeable effect being an increased width of the lower L_2 component. The effects of crystal fields at low symmetry core-hole sites are also considered. We show that it is essential to treat the exchange part using the full core-valence exchange operator in order to describe the crystal fields in a satisfactory manner.

Temperature effects on surface core level spectra

Stefano de Gironcoli
INFM-DEMOCRITOS and Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

I report on some recent ab-initio studies on the effects of temperature on the peak position and width of core level spectra for metallic surfaces. Calculations for the vibrational broadening of core level peaks in Be(0001) and Rh(001) will be presented. Calculation reproduces very well the multi-phonon replicas recently observed in low-temperature high-resolution photoemission spectra emerging from bulk and inner surface layers in Be(0001). The absence of marked multi-phonon replicas in the photoemission spectrum from the topmost surface layer is traced back to a stronger lattice relaxation around surface core-hole defect and to its coupling to surface phonons.

Moreover by comparing recently measured temperature-dependent surface core level shifts and surface state positions to values calculated with Density Functional Theory for different surface geometries it has been possible to determine the multilayer thermal expansion of the first three interlayer spacings of the (0001) surface of beryllium. These results reveal that, in the temperature range from 300 to 700 K the first-to-second, second-to-third and third-to-fourth interlayer distances expand by 88 ± 15, -10 ± 15 and -6 ± 20 $\times 10^{-6}$ K^{-1}, respectively. This work confirms a previous Low Energy Electron Diffraction study which

reported a strong thermal surface expansion in Be(0001) but it is in disagreement with the most advanced theoretical calculation available at present.

In Rh(001) the comparison of calculated position and vibrational broadening of layer-specific core level peaks with experimental temperature-dependent photoemission spectra allows to show the composite nature of the supposedly bulk peak. These findings have been confirmed by recent experimental work.

Quasiparticle band structure of the As vacancy on GaAs(110)

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We report *ab initio* calculations of the structural and electronic properties of the As vacancy on GaAs(110). Emphasis is put on accurate convergence testing of atomic relaxations and the energy of the defect levels and their dispersion with respect to surface cell size and k-point sampling. Under p-type conditions the stable charge state of the vacancy is predicted to be +1 in agreement with other calculations and experiment.

The vacancy introduces two defect levels in the band gap. Since an LDA description for states in the band gap is insufficient we address this problem by performing GW calculations. We focus on the lower of these states, which may be unoccupied, singly or doubly occupied depending on the position of the Fermi level. This defect state consists of Ga-Ga bonds which are not present in neither the bulk nor the clean surface. As a consequence we found the GW corrections to be non-trivial and different from the corrections to the bulk band gap.

The energy of the defect level is extracted at the special k-point and the accuracy of this procedure is evaluated by a tight-binding fit to the *ab initio* calculated dispersion relations.

Ab initio calculation of the anisotropic dielectric tensor of GaAs/AlAs superlattices

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The size reduction achieved in one, two or three dimensions in heterostructures at the nanoscale level leads to electronic ground and excited states widely different from those of the bulk crystals, and has opened the way to a new generation of optoelectronic and photonic devices. GaAs/AlAs superlattices (SL's) are extensively studied examples. While the GaAs and AlAs bulk semiconductors present an isotropic optical response, in the GaAs/AlAs SL the lowering in the crystal symmetry gives rise to an optical anisotropy.

Here, we will present a study of the dielectric tensor of (001) $(GaAs)_p/(AlAs)_p$ SL's as a function of their period p for $1 \leq p \leq 12$, starting from Density Functional Theory. We have performed both *ab initio* [1] and semi-empirical calculations [2], and we will compare their results. The simple picture of the macroscopic dielectric function being a sum of independent transitions between one-electron states ignores contributions which may be especially important when the scale of the system is reduced and the inhomogeneity of the medium more pronounced. In particular, the crystal local field effects are expected to be relevant, since they reflect the charge inhomogeneity of the responding material. This point turns in fact to be crucial for the explanation of the SL birefringence, as we will illustrate by discussing the following results: - Calculations neglecting local field effects account neither for the experimentally observed value of the static birefringence [4], nor for its decrease with decreasing SL period p, even qualitatively. - The behavior of the dielectric tensor is determined by the interplay between quantum confinement and the local fields effects. The use of the effective medium approach [3] is shown to be justified in the growth direction even for small periods, whereas the direct effect of quantum confinement is found to be larger in the in-plane direction. - The static birefringence is drastically enhanced by the anisotropy of the local fields. Including the latter, the *qualitative* behavior of the experiment [4] can be reproduced. The *quantitative* agreement is improved by the inclusion of further many-body effects, using the Slater-Koster contact exciton model [5].

[1] S. Botti, N. Vast, L. Reining, V. Olevano, L. C. Andreani (submitted).

[2] S. Botti and L. C. Andreani, Phys. Rev. B **63**, 235313 (2001).

[3] D. Bergman, Physics Report **43**, 291 (1978); M. G. Cottam and D. R. Tilley, in *Introduction to surface and superlattice excitations* (Cambridge University Press, Cambridge, 1989), p. 267; E. Jahne, phys. stat. sol. (b) **194**, 279 (1996).

[4] A. A. Sirenko, P. Etchegoin, A. Fainstein, K. Eberl, and M. Cardona, Phys. Rev. B **60**, 8253 (1999).

[5] J. E. Rowe and D. E. Aspnes, Phys. Rev. Lett. **25**, 162 (1970).

Ab initio calculations of the dielectric response of graphite and small-diameter carbon nanotubes

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The dielectric response functions and optical absorption spectra of graphite and of small-diameter carbon nanotubes (4 Å) were determined within the framework of time-dependent density-functional theory in both the RPA and adiabatic LDA approximations.

For graphite, the dispersion of the two valence plasmons and, in general, the lineshape of the electron-hole excitation continuum in the loss spectrum was determined for a wide

range of momentum-transfer orientations with respect to the basal planes. Our findings show important anisotropic behavior of the dielectric response and strong effects of the interlayer Coulomb interaction on the loss spectra, notably on the frequency of the higher-frequency $\pi + \sigma$ plasmon. Incorporation of local fields in the response has an important influence on the spectra for momentum orientations approaching the crystallographic c-axis direction [1]. Similarly, the calculated spectra of the small tubes display strong anisotropy and dependence on the inter-tube interaction.

[1] A. G. Marinopoulos, L. Reining, V. Olevano, A. Rubio, T. Pichler, X. Liu, M. Knupfer, and J. Fink, Phys. Rev. Lett., to appear (2002).

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5.2 ESF Workshop/Conference Announcements

5.2.1 VASP Hands-on Course

Workshop announcement

Hands-on tutorial course on the Vienna ab-initio simulation package VASP

A hands-on tutorial workshop introducing the Vienna ab-initio simulation package VASP for ab-initio simulations of materials properties and processes will be held at Vienna University on February 10–13, 2002. The workshop will be organized by the Institut for Materials Physics of Vienna University and the Research Center and Science College "Computational Materials Science" (CMS), in cooperation with Materials Design Sarl, LeMans (France).

Scientific scope of the workshop:

The Vienna ab-initio simulation program VASP, based on either pseudopotential or projector-augmented-wave (PAW) approaches, has established itself as one of the most efficient and widely used tools for performing ab-initio density functional calculations. Currently about 400 academic and industrial research groups are using VASP for their work.

Although the program is well documented, the access to these techniques is sometimes found a bit difficult by people with no background in density-functional calculations. The purpose of this workshop is to offer an introduction to the fundamentals of ab-initio density functional theory, of pseudopotentials, PAW's and large scale calculations, as well as a practical hands-on training for young students and non-specialists. Particular emphasis will be laid on a thorough discussion of the problems that can be solved directly with the basic code (and the tools implemented in it) and on the definition of the interface to other tools. The hands-on training will be based on a LINUX platform (Pentium PC's with 512MB memory), but a short introduction to the use of VASP on an NT-Windows platform, using the MEDEA environment developed by Materials Design will be offered as well. Participants of the workshop belonging to academic institutions (doctoral students and young post-docs) will receive a free personal licence to VASP. Detailed informations on the workshop program can be found on the web-page **http://cms.mpi.univie.ac.at/vasp-workshop**

Attendance:

The participants are expected to come mostly from areas where the used of DFT techniques is not yet current practice: materials engineering, mineralogy, geophysics, ... but also from experimental physics and chemistry. The number of particpants will be limited to about forty. Familiarity with LINUX is mandatory, a thorough background in solid state theory and quantum mechanics is expected. For students and post-doc's a recommendation from the supervisor will be appreciated. An application form can be found on the homepage of the workshop (http://cms.mpi.univie.ac.at/vasp-workshop). The form should be completed and returned as soon as possible to the workshop secretary, either by email (tina.branis@univie.ac.at) , by fax (+43-1-4277-9514) or by ordinary mail to the address given below. Early registration is recommended. Preference will be given to doctoral students and young post-docs meeting, the requirements on a first come, first serve basis.

Funding: The workshop is sponsored by the Ψ_k-Research Programme *Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces* of the European Science Foundation. There is no workshop fee. On request, part of the local expenses can be covered out of the funds provided by the ESF. Travel expenses will be at the charge of the participants, only in very exceptional cases a contribution to the travel expenses will be possible.

Organizers:

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6 General Workshop/Conference Announcements

6.1 ELEVENTH INTERNATIONAL WORKSHOP COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE TOTAL ENERGY AND FORCE METHODS

16 - 18 January 2003
Miramare, Trieste, Italy

As in previous meetings of this series, the Workshop will be devoted to recent advances in computational condensed matter physics, based on realistic calculations of the electronic structure of polyatomic systems.

The activity is hosted at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, and is co-sponsored by the ICTP, the DEMOCRITOS National Simulation Center of the Italian Istituto Nazionale per la Fisica della Materia (INFM), and by the International School for Advanced Studies (SISSA).

Thanks to sponsorship from the European Community, under the High-level Scientific Conferences programme, a limited number of participation grants are available for young European or Associated Nation participants.

Information on the program, registration procedure, etc. can be found on the web at URL:

http://www.democritos.it/totalenergy

We look forward to seeing you in Trieste next January!

Richard M. Martin
Michael W. Finnis
Stefano Baroni

6.2 Joint DEMOCRITOS - ICTP Winter College on Numerical Methods in Electronic Structure Theory

16 January - 4 February 2003
Miramare - Trieste, Italy

An international course on pseudopotential plane-wave electronic structure calculations will be held at the Abdus Salam International Centre for Theoretical Physics, (ICTP), Trieste, Italy, from 20 January to 4 February 2003, with the co-sponsorship of the INFM DEMOCRITOS National Simulation Center.

DIRECTORS:

Stefano Baroni - Scuola Internazionale Superiore di Studi Avanzati (SISSA) and DEMOCRITOS, Trieste
Andrea Dal Corso - SISSA and DEMOCRITOS
Stefano de Gironcoli - SISSA and DEMOCRITOS
Paolo Giannozzi - Scuola Normale Superiore, Pisa, and DEMOCRITOS, Trieste

PURPOSE AND NATURE

This college aims at a general introduction to electronic structure calculations within Density Functional Theory and using the plane-wave pseudopotential method. The focus will be on the physical principles and numerical algorithms which underlie the implementation of state-of-the-art computer codes. The College will be opened by the "Eleventh International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods" which all the participants of the College are invited to attend. A series of theoretical lectures will then follow, aimed at illustrating how an electronic structure computer code is developed in practice. These lectures will be complemented by hands-on computer sessions where it will be demonstrated how a simple and fully operational plane-wave pseudopotential computer code is developed, starting from scratch. Advanced topics such as first-principles molecular dynamics and the implementation of density-functional perturbation theory will also be covered. Finally, in the last part of the college, a state-of-the art open-source pseudopotential package (PWSCF) will be distributed to the participants and a series of tutorials will be held to illustrate its usage with a number of currently significant applications.

PARTICIPATION

Students and young scientists from all countries that are members of the UN, UNESCO or IAEA can apply to participate in the College. This college is specially targeted to strongly motivated graduate students and young post-doctoral scientists. Prior specific training in electronic structure calculations is not strictly required. However, participants are expected to have a good working knowledge of elementary quantum mechanics and solid state physics. Some knowledge of FORTRAN-90 and UNIX is a prerequisite. As the College will be conducted in English,

participants should have an adequate working knowledge of that language.

There is no participation fee, however, participants from developed countries are expected to cover their own travel and living expenses. A limited number of grants to support the participation of young Italian scientists will be provided by the INFM DEMOCRITOS National Simulation Center. Financial support has also been obtained from the European Community to promote participation of young European Community (EC) or Associated Nation (AN) researchers to the "Eleventh International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods" which opens the present activity. Prospective participants wishing to apply for such support must make an explicitly mention in their application form.

Those wishing to participate should complete the request for participation form (to be found on the web at url:

http://www.democritos.it/wintercollege) and return it to the secretary

of the college, Ms. Gabriella De Meo, at the address: smr1492@ictp.trieste.it. Although there is no formal deadline for applications from scientists who do not require a visa, the number of positions available to scientists from developed contries is limited, and applications will be processed on a first-come first-served basis.

Preliminary List of Lecturers

* All the speakers of the "XI International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods" (see http://www.democritos.it/totalenergy)

* Stefano Baroni, SISSA and DEMOCRITOS-INFM, Trieste, Italy
Andrea Dal Corso, SISSA and DEMOCRITOS-INFM, Trieste, Italy
Paolo Giannozzi, SNS, Pisa, and DEMOCRITOS-INFM, Trieste, Italy
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Nicola Marzari MIT, Boston, USA
Giorgio Pastore University of Trieste and DEMOCRITOS-INFM
Marco Saitta Universit Pierre et Marie Curie, Paris, France

Details of the program will be will be posted on

http://www.democrits.it/wintercollege, as soon as available.

6.3 JOINT CCP3/CCP5 WORKSHOP ON NANOSCALE MODELLING

Queens' College, Cambridge, 6-7 January, 2003

CCP3 and CCP5 (with support from the IRC in Nanotechnology, the EPSRC Network on Theory and Experiment in Extreme Nanotechnology, and the Thin Films and Surfaces Group of the Institute of Physics) are organizing a joint workshop on the modelling and simulation of nanostructures. We wish to confront theorists and modellers with experimental facts and problems, as well as the latest developments in their own fields.

The meeting will take place in Queens' College, Cambridge on 6-7 January 2003, starting after lunch on Monday 6 Jan and finishing after lunch on Tuesday 7 Jan. There will be oral sessions (principally invited talks) plus a contributed poster session early on Monday evening. Accommodation will be available in the college. Numbers will be limited to approximately 70 participants; places will be allocated mainly on a first-come, first-served basis, but with a preference to those wishing to present a poster.

The approximate cost of attendance will be as follows:

Resident, en suite: 80.00 GBP
Resident, shared bathroom: 60.00 GBP
Non-resident (includes all meals except breakfast): 20.00 GBP

Invited speakers include: Malcom Green (Oxford), Alan Windle (Cambridge), Mads Brandbyge (Lyngby), Richard Palmer (Birmingham)*, Tchavdar Todorov (QUB)* Mark Ratner(Northwestern)*

* Subject to final confirmation

Andrew Fisher (mailto:andrew.fisher@ucl.ac.uk)
John Harding (mailto:j.harding@ucl.ac.uk)

FUNDAMENTAL PHYSICS OF FERROELECTRICS: FERRO2003

Williamsburg, Virginia, U.S.A.

2-5 February, 2003

http://cst-www.nrl.navy.mil/~singh/ferro2003

SECOND ANNOUNCEMENT AND CALL FOR PAPERS

Fundamental Physics of Ferroelectrics provides a forum for the discussion of forefront theoretical and experimental research on ferroelectricity and ferroelectric materials. Invited speakers (not all confirmed yet) include:

L. Bellaiche, University of Arkansas
R. Blinc, J. Stefan Institute
B. Burton, NIST
W. Cao, Pennsylvania State University
G. Ceder, MIT
H. Chen, University of Illinois
R. Cohen, Geophysical Laboratory
W. Kleemann, Uni. Duisburg
S. O'Brien, Columbia University
C. Randall, Pennsylvania State University
A. Rappe, University of Pennsylvania
E. Salje, University of Cambridge
G. Samara, Sandia National Laboratory
J. Scott, University of Cambridge
G. Shirane, Brookhaven National Labooratory
J. Toulouse, Lehigh University
D. Viehland, Virginia Tech
M. Weissman, University of Illinois

The workshop will consist of oral sessions containing invited and contributed talks as well as a poster session. Presenters are encouraged to leave ample time for discussion at the end of their talks in keeping with the workshop format. A proceedings will be published, as in past years.

Deadlines are:

Housing and Registration: Dec. 18, 2002.

Abstracts: Dec. 30, 2002.

For details please see the web-site:

`http://cst-www.nrl.navy.mil/~singh/ferro2003`

David J. Singh, NRL
Peter K. Davies, University of Pennsylvania

European Material Research Society

Strasbourg (France) June 10-13, 2003

Symposium K

Design, Characterisation and Modelling of Molecule-Based Magnetic Materials

See web-site: http://www-emrs.c-strasbourg.fr for abstract submission.

Among the topics:

Molecular and Solid-State Engineering
Molecular Magnets
Nanomaterials and Low Dimensional Materials
Multiproperty Materials
Recent progresses in physical characterization
Theory and Modelling:
Electronic structure advances
Magnetic models
Devices and applications

For information write to Pierre.Rabu@ipcms.u-strasbg.fr

6.6 Conference on "Modelling of Materials: Atomistic and Ab Initio Approaches"

First Annoucement

Mansfield College, Oxford University, UK

9-10 April, 2003

http://www.tc.bham.ac.uk/~roy/TCG/Materials.html

7 General Job Announcements

POSTDOCTORAL POSITION: Proton Transfer in Biosystems Bochum University, Germany

Applications are invited for a research associate position. The preferred starting date would be spring 2003.

The ideal candidate would have significant experience in mixed quantum/classical, Car-Parrinello, and/or path integral simulations. She or he would work primarily on quantum simulations of proton transfer along hydrogen-bond networks in complex biological systems.

In addition, a PhD position in electronic structure theory (surface science, heterogeneous catalysis, theoretical STM imaging) is expected to become available in July/August 2003.

The Theoretical Chemistry Group at RUB offers an exciting interdisciplinary environment with excellent working conditions including a 500 GFLOPS parallel machine. The techniques used and developed in the Marx group are covered in

http://www.theochem.ruhr-uni-bochum.de/go/cprev.html

and additional information can be obtained from the home page.

Candidates should send a detailed CV and contact information for academic references to ¡office@theochem.ruhr-uni-bochum.de¿. Consideration of candidates will begin immediately and continue until the position is filled. The University particularly welcomes applications from women.

Professor Dominik Marx
Lehrstuhl fuer Theoretische Chemie
Ruhr-Universitaet Bochum
44780 Bochum, Germany

Phone : ++49 234 322 6485
Fax : ++49 234 321 4045
office@theochem.ruhr-uni-bochum.de

http://www.theochem.ruhr-uni-bochum.de/

Postdoctoral Position in Computational Chemistry/Biochemistry
Institute of Microstructural Sciences, National Research Council of Canada

Applications are invited for a postdoctoral fellow position in an area of computational chemistry/biochemistry or related field. The applicant should have a strong background in quantum mechanics and molecular dynamics methods and should be familiar with first principles and empirical modelling software.The project will involve simulating molecular recognition in polymers/biopolymers with applications in biosensing and is part of a collaboration led by the Institute of Microstructural Sciences, National Research Council of Canada. Prior experience in modelling of biological systems is an asset and a motivation for working in close collaboration with experimentalists is important.

The position is available beginning January 1, 2003, initially for one year with possible extension for a second year subject to mutual agreement. The candidates are invited to send their applications consisting of a curriculum vitae and a list of publications and should arrange to have three letters of recommendation sent to:

Jolanta B. Lagowski
Dept. of Physics and Physical Oceanography
Memorial University of Newfoundland
St. John's, Newfoundland
A1B 3X7

phone: 709 737-2667
fax: 709 737-8739
email: jolantal@physics.mun.ca

Postdoctoral Position
University of California, Davis

We have a postdoctoral position available immediately to conduct research in the area of spintronics. Experience in the computation of electronic structure based on density functional theory is required, and experience with established computer codes designed to work with large systems, such as VASP, SIESTA, etc., is highly desirable. Experience in other techniques related to spintronics is desirable. The appointment is expected to be for two years. Candidates should contact one of the persons below for further information. Research will be carried out at the University of California Davis.

Prof. Ching Y. Fong (fong@physics.ucdavis.edu)
Prof. Warren Pickett (pickett@physics.ucdavis.edu)

Postdoctoral Research Position in Computational Materials Physics

National Renewable Energy Laboratory, Golden, Colorado

We at the National Renewable Energy Laboratory (one of the DOE's prestige National Laboratories near Denver, the gate to the beautiful Rocky Mountains and ski resorts) invites applications for a theoretical postdoctoral position, available in April 2003. Initial assignment is for a year, but renewable upon funding availability, performance, and mutual agreement up to a total of three years. The research direction is to develop first-principles theories for the next-generation semiconductors for optoelectronic and nanoscience applications. Some recent work include wide-gap materials such as p-type zinc oxide, n-type diamond, ultrahigh carrier-density silicon, visible light-emitting silicon, and tunable bandgap gallium arsenide nitride. The starting salary is USD 42-50K/year depending on qualification. Candidate should send a curriculum vitae, list of publications (including preprints of unpublished papers, if possible) and arrange three reference letters to

Dr. Shengbai Zhang
National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401, USA
Email:szhang@nrel.gov

NREL is an equal opportunity/affirmative action employer.

PhD position

Electronic Structure Calculation

Computational Modelling Group

NMRC, Unversity College, Cork, Ireland

A PhD studentship is available in the Computational Modelling Group at the NMRC, Unversity College, Cork, Ireland. Candidates with a primary degree in physics, chemistry, computational materials science, or a related discipline and with a strong interest in molecular physics are invited to apply.

With modern electronic structure techniques, it is possible to model the ground state properties of molecules and materials with high accuracy, but prediction of electronic excitations remains a computational challenge. This project aims to accurately calculate the vertical excitation energies of small and medium sized molecules. The project will involve the application of electronic structure theory, including electron correlation, through the application of modern quantum mechanical computer programs. We use a method for the calculation of excitation energies that allows the user to choose the level of accuracy for treatment of electronic correlation. The goal of the project is to investigate the balance between ground and excited state calculations to achieve precise, yet computationally efficient, calculations for excited state energies. Our method has been demonstrated to work well for atomic excitations.

The NMRC houses ca. 60 graduate students in areas ranging from nanotechnology and optoelectronics to microelectronics, and ICT/Life sciences, and ca. 150 staff members (http://www.nmrc.ie/). The centre is equipped with modern computer facilities and laboratories. We are involved in national and international research projects and we encourage our students to actively partake in these collaborations. The successful candidate is allowed to register for the PhD programmes in either the Department of Physics, Chemistry or Microelectronics, based upon the candidate's preference and background.

For informal enquiries contact Andreas.Larsson@nmrc.ie or Jim.Greer@nmrc.ie.

Fellowships available at Isfahan University of Technology, Iran

The computational condensed matter group physics department of Isfahan University of Technology (IUT) is going to expand its regional scientific activity by acting as an ICTP Affiliated Centre. Following such a mission, the Abdus Salam International Centre for Theoretical Physics (ICTP) and IUT have agreed to support the below mentioned fellowships for the year 2003:

1) Two Fellowships for young researchers (possessing a PhD degree or at the final stages of getting it) from the regional countries (Western South Asia, Central Asia, and Middle East) to come and work in the center as long term visitors (3-6 months).

2) Two Fellowships for senior researchers from the regional countries to come and work in the center as short term visitors (4-12 weeks).

The applicants are expected to have a keen interest in computational condensed matter physics, with some hands on experience on first principle methods.

The fellowships are available from 1st of January 2003.

Applications including, a full CV, a list of publications, an abstract of her/his research achievements (within one page of an A4 sheet), a proposal of about 500 words explaining the details of the research project that the applicant is going to perform during the stay in the center, and names and addresses (email) of two or three referees should be sent to the following address:

Professor Hadi Akbarzadeh
Department of Physics,
Isfahan University of Technology,
Isfahan, Iran
email: akbarzad@cc.iut.ac.ir,
Tel: +98-311-3912375 (or 3913700),
fax: +98-311-3912376.

Accepted candidates are entitled for the following supports:

1. Travel expenses by economy round trip air ticket.

2. Accommodation in IUT Guest House.

3. 400 Euro per month for living expenses (For senior researchers it can be increased to 500 Euro).

4. One full meal per day.

Current research interests of the center:

Electronic structure calculations, as a valuable tool for understanding the properties of condensed matter, are the main current activity in the computational condensed matter group in

physics department of Isfahan University of Technology. Our calculations are within the density functional theory using FP-LAPW method. We have access and hands on experience to work with WIEN2k code (www.wien2k.at). This general purpose electronic structure code is a very appropriate tool to calculate many properties of a solid: band structure, density of states, equilibrium geometry, magnetic structure, electric-field gradients, hyperfine fields, and X-ray spectra, etc. The code contains LDA+U to study highly correlated systems.

The ongoing research projects in the group are as follow:

1. Structural, electronic and magnetic properties of MnAs.

2. Structural and electronic properties of CeFe2.

3. Investigation the valency of rare earth elements in RIn3 and RSn3: Ab initio analysis of electric field gradients

4. Investigation of the valency of Actanides in USn3, UIn3, and NpIn3 by ab-initio methods.

5. First principle calculation of hyperfine fields and local relaxation at 4d and 5sp impurities in bcc Cr.

POST-DOCTORAL POSITIONS AT THE INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS (ICTP)

TRIESTE, ITALY

Post-doctoral positions will be available in the Condensed Matter Group of the International Centre for Theoretical Physics (ICTP), Trieste, Italy, starting Spring and Fall 2003. The appointments will be for one year, renewable for a second year. A background in electronic structure calculations and/or molecular dynamics is required. Areas of interest include high-pressure transformations and surface physics/chemistry. Details at `http://www.ictp.trieste.it/~scandolo/post-do`
Please contact Sandro Scandolo (scandolo@ictp.trieste.it) for further information.

Two PhD Positions

in Group for Theoretical Solid State Physics Leibniz-Institute for Solid State and Materials Research (IFW) Dresden

http://www.ifw-dresden.de

The Group for Theoretical Solid State Physics at the Institute for Solid State and Materials Research Dresden invites applications for two PhD positions. Both positions are attached to the 'Sonderforschungsbereich 463', a joined project established at Technische Universitaet Dresden and financed by the German Science Foundation. The research field of this project is Structure, Magnetism, and Transport on Rare Earth – Transition Metal Compounds.

Position (i) is devoted to the Electronic Structure and Super-conductivity of Anisotropic Multi-band Super-conductors. In particular, the following topics are addressed:
- realistic treatment of Fermi surface integrals in the strong coupling theory of super-conductivity;
- influence of co-existing magnetic order;
- collaboration with experimental groups (evaluation of the magnetic and crystal field excitations that will be measured by inelastic neutron scattering).

Position (ii) is devoted to the Density Functional Theory of Magnetic and Spectroscopic Properties. In particular, the following topics are addressed:
- magnetic properties and electronic structure in the bulk and at the surface of rare earth – transition metal compounds;
- evaluation of exchange coupling and crystal field interaction;
- magneto-elastic properties.

Both projects will be carried out in close collaboration with other, in particular experimental, groups at IFW, University of Technology Dresden, Max-Planck-Institute for Physics of Complex Systems, and Max-Planck-Institute for Chemical Physics of Solids.

Salaries will be based on 75% BAT IIa-O, annual net income about 12-15 KEUR, depending on age and social status.

At the moment, the Group for Theoretical Solid State Physics consists of eleven scientists in solid state theory, three PhD students, and up to ten guest scientists. The group has up-to-date computer facilities, daily coffee meetings, and a lively exchange with a number of other groups worldwide (theoretical and experimental, physics and chemistry). The city of Dresden is situated mid-way between Berlin and Prague, in the valley of river Elbe. With a population of about 500,000, it is known for a rich cultural live and for its baroque silhouette.

Interested candidates should send their curriculum vitae, related documents, a brief statement

about previous research activities, and 1-2 references to:

Dr. Manuel Richter
Institute for Solid State and Materials Research
P.O. box 270 116
D-01171 Dresden
Germany
email: m.richter@ifw-dresden.de

Postdoctoral Position in Electronic Structure Applied to Spin-Dependent Properties in Semiconductors Case Western Reserve University

A post-doctoral position is available immediately in the group of Prof. Walter Lambrecht in the Department of Physics, Case Western Reserve University, Cleveland, Ohio. The main focus of the work will be development of computational methods for magneto-optics in hybrid magnetic material/semiconductor structures and magnetic semiconductors. Familiarity with first-principles computational methods is expected. Experience with code development is desirable.

Please, send a CV, along with names and contact information for 2-3 references to lambrecht@cwru.edu. Pdf format is preferred but not required. Consideration of candidates will start immediately and will continue until the position is filled. For further information, contact:

Prof. Walter R. L. Lambrecht
Department of Physics
Case Western Reserve University
10900 Euclid Avenue
Cleveland, OH 44106-7079
U.S.A
Phone: +(216) 368-6120
Fax: +(216) 368-4671
Email: lambrecht@cwru.edu
Website: http://els3.phys.cwru.edu/

8 Abstracts

Neutral-ionic phase transition : a thorough ab-initio study of TTF-CA

V. Oison[1], C. Katan[1], P. Rabiller[1], M. Souhassou[2] and C. Koenig[1]
[1] *Groupe Matière Condensée et Matériaux,UMR6626 CNRS - Université Rennes 1, Campus de Beaulieu Bât. 11A, F-35042 Rennes Cedex, France*
[2] *LCM^{3}B, UMR7036 CNRS - Université Henri Poincaré Nancy 1, F-54506 Vandœuvre lès Nancy, France*

Abstract

The prototype compound for the *neutral-ionic* phase transition, namely TTF-CA, is theoretically investigated by first-principles density functional theory calculations. The study is based on three neutron diffraction structures collected at 40, 90 and 300 K (Le Cointe et al., Phys. Rev. B **51**, 3374 (1995)). By means of a topological analysis of the total charge densities, we provide a very precise picture of intra and inter-chain interactions. Moreover, our calculations reveal that the thermal lattice contraction reduces the indirect band gap of this organic semi-conductor in the neutral phase, and nearly closes it in the vicinity of the transition temperature. A possible mechanism of the *neutral-ionic* phase transition is discussed. The charge transfer from TTF to CA is also derived by using three different technics.

(submitted to Phys. Rev. B)
Manuscripts available from: http://xxx.lanl.gov/abs/cond-mat/0210017
Contact person: Claudine.Katan@univ-rennes1.fr

Magnetic circular dichroism in X-Ray Resonant Raman Scattering in perpendicular geometry from $CoFe_2O_4$ and Co metal: comparison between valence and inner-shell channels

L. Braicovich
Politecnico di Milano, Italy
G. van der Laan
Daresbury Laboratory, UK
G. Ghiringhelli
Politecnico di Milano, Italy
A. Tagliaferri
Politecnico di Milano, Italy
N. B. Brookes
ESRF, France

Abstract

We present results on resonant Raman scattering (RRS) in perpendicular geometry excited with circularly polarized x-rays at the Co $L_{3,2}$ edges in $CoFe_2O_4$ (Co ferrite) and Co metal. In this geometry the incident x-ray beam is perpendicular to the magnetization and the magnetic dichroism is only present in the RRS and not in the absorption. We compare the $3s$-RRS channel terminating in an inner shell $3s$ hole and extra $3d$ electron ($2p^6 3d^n \rightarrow 2p^5 3d^{n+1} \rightarrow 2p^6 3s^1 3d^{n+1}$) and the 3d-RRS channel ending in a $3d$ electron-hole pair ($2p^6 3d^n \rightarrow 2p^5 3d^{n+1} \rightarrow 2p^6 3d^n$). The work is based on the measurement of the spectra vs incident photon energy and integrated over the scattered photon energy. In both samples the dichroism of the inner-shell channel is an order of magnitude larger than that of the valence channel. The result is explained by a theory based on the fast-collision approximation. We show that this theory provides a general way to choose the optimum scattering channel in the study of magnetic dichroism in perpendicular geometry. The impact of the results is briefly discussed.

(Physical Review B, issue of 1st November, 2002)
Contact person: g.vanderlaan@dl.ac.uk

Pressure-induced structural transitions in MgH_2

P. Vajeeston, P. Ravindran, A. Kjekshus, and H. Fjellvåg
Department of Chemistry, University of Oslo, Box 1033, Blindern, N-0315, Oslo, Norway.

Abstract

The stability of MgH_2 has been studied up to 20 GPa using density-functional total-energy calculations. At ambient pressure α-MgH_2 takes a TiO_2-rutile-type structure. α-MgH_2 is predicted to transform into γ-MgH_2 at 0.39 GPa. The calculated structural data for α- and γ-MgH_2 are in very good agreement with experimental values. At equilibrium the energy difference between these modifications is very small, and as a result both phases coexist in a certain volume and pressure field. Above 3.84 GPa γ-MgH_2 transforms into β-MgH_2; consistent with experimental findings. Two further transformations have been identified at still higher pressure: i) β- to δ-MgH_2 at 6.73 GPa and (ii) δ- to ϵ-MgH_2 at 10.26 GPa.

(Published in Phys. Rev. Lett., **89**, 175506 (2002))
Contact person: ravindran.ponniah@kjemi.uio.no

Violation of "the 2 Å rule" for metal hydrides

P. Ravindran, P. Vajeeston, R. Vidya, A. Kjekshus, and H. Fjellvåg
Department of Chemistry, University of Oslo, Box 1033, Blindern, N-0315, Oslo, Norway

Abstract

Using gradient-corrected, all-electron, full-potential, density-functional calculations, including structural relaxations, it is found that the metal hydrides $RT\mathrm{InH}_{1.333}$ (R = La, Ce, Pr, or Nd; T = Ni, Pd, or Pt) possess unusually short H−H separations. The most extreme value (1.454 Å) ever obtained for metal hydrides occurs for $\mathrm{LaPtInH}_{1.333}$. This finding violates the empirical rule for metal hydrides, which states that the minimum H−H separation is 2 Å. Electronic structure, charge density, charge transfer, and electron localization function analyses on $RT\mathrm{InH}_{1.333}$ show dominant metallic bonding with a non-negligible ionic component between T and H, the H−H interaction being weakly metallic. The paired, localized, and bosonic nature of the electron distribution at the H site are 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. Also, R−R interactions contribute to shielding of the repulsive interactions between the H atoms.

(Published in Phys. Rev. Lett., **89**, 106403 (2002))
Contact person: ravindran.ponniah@kjemi.uio.no

Antiferromagnetic vs ferromagnetic interactions and spin-glass-like behavior in ruthenates

P.Ravindran, R.Vidya, P.Vajeeston, A.Kjekshus, and H.Fjellvåg
Department of Chemistry, University of Oslo, Box 1033, Blindern, N-0315, Oslo, Norway

Abstract

We have made a series of gradient-corrected relativistic full-potential density-functional calculation for Ca-substituted and hole-doped $SrRuO_3$ in para, ferro, and *A*-, *C*-, and *G*-type antiferromagnetic states. Magnetic phase-diagram data for $Sr_{1-x}Ca_xRuO_3$ at 0 K are presented. Neutron diffraction measurement combined with total energy calculations show that spin-glass behavior with short-range antiferromagnetic interactions rules in $CaRuO_3$. The substitution of Sr by Ca in $SrRuO_3$ decreases the ferromagnetic interaction and enhances the *G*-type antiferromagnetic interaction; the *G*-AF state is found to stabilize around $x = 0.75$ consistent with experimental observations. Inclusion of spin-orbit coupling is found to be important in order to arrive at the correct magnetic ground state in ruthenates.

(Published in Solid State Commun. **124**, 293 (2002))
Contact person: ravindran.ponniah@kjemi.uio.no

Ab initio theory of phase transitions and thermoelasticity of minerals

Artem R. Oganov, John P. Brodholt, G. David Price
University College London, Gower Street, London WC1E 6BT, U.K.

Abstract

Accurate quantum-mechanical simulations have significantly extended the current picture of the Earth and hold a great promise for the future of the Earth and planetary sciences. Studies of phase transitions, equations of state, elasticity and thermoelastic properties of the Earth-forming minerals are essential to geophysics. This chapter gives a basic background of the physics of the deep Earth and outlines the theory of phase transitions, equations of state, elasticity and thermoelastic properties. A particular emphasis is put on the principles of quantum-mechanical simulations and some recent results relevant to geophysics.

(Chapter in: EMU Notes in Mineralogy, v.4 Energy Modelling in Minerals, edited by C.M. Gramaccioli, Budapest: Eotvos University Press (in press))
For reprints contact A.R. Oganov: a.oganov@ucl.ac.uk

All-electron and pseudopotential study of MgO: equation of state, anharmonicity, and stability

Artem R. Oganov (1) and Peter I. Dorogokupets (2)
(1) Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, U.K.
(2) Institute of the Earth's Crust, 128 Lermontov Street, 664033 Irkutsk, Russia

Abstract

We have studied the high-pressure behaviour of periclase (MgO) using density functional simulations within the generalized gradient approximation (GGA). The static and thermal (P-V-T) equation of state, B1-B2 transition pressure, elastic constants, Grneisen parameter, and the intrinsic anharmonic parameters were calculated from static and ab initio molecular dynamics simulations. The simulations were performed using the projector augmented-wave (PAW) and pseudopotential methods with different descriptions of the Mg atom (small-core and large-core). We find large discrepancies between the results of large-core pseudopotential calculations and the more accurate PAW and small-core pseudopotential calculations. The errors for large-core pseudopotentials increase with pressure and are mainly due to the overlap between the Mg semicore (2p-) orbitals and the valence orbitals, both of the same Mg atom and of the neighbouring O atoms, rather than core polarization or core-core overlap effects. In agreement with previous works, we conclude that MgO remains in the B1 (NaCl) structure at all pressures existing within the Earth. The transition from the NaCl-type to the CsCl-type structure is predicted to occur at 509 GPa. We find that the static equation of state is better described by the 3rd-order Birch-Murnaghan function than by the Vinet function. Direct ab initio calculations avoid the simplifying assumptions inherent to many empirical treatments of thermoelasticity and allowed us to assess some of the common assumptions. We present a detailed quantitative analysis of the effects of intrinsic anharmonicity and analyse the validity of the Mie-Grneisen approximation at high temperatures.

(Phys. Rev. B, submitted)
For preprints contact A.R. Oganov: a.oganov@ucl.ac.uk

Computational mineral physics and the physical properties of perovskites

Brodholt J.P., Oganov A.R., Price G.D.
Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, UK

Abstract

The inherent uncertainties in modern first-principles calculations are reviewed using geophysically relevant examples. The elastic constants of perovskite at lower-mantle temperatures and pressures are calculated using ab initio molecular dynamics. These are used in conjunction with seismic tomographic models to estimate that the lateral temperature contrasts in the Earth's lower mantle are 800 K at a depth of 1000 km, and 1500 K at a depth of 2000 km. The effect of Al3+ on the compressibility of MgSiO3 perovskite is calculated using three different pseudopotentials. The results confirm earlier work and show that the compressibility of perovskites with Al3+ substituted for both Si4+ and Mg2+ is very similar to the compressibility of Al3+-free perovskite. Even when 100with Al3+, the bulk modulus is only 7perovskite. In contrast, perovskites where Al3+ substitutes for Si4+ only and that are charge balanced by oxygen vacancies do show higher compressibilities. When corrected to similar concentrations of Al3+, the calculated compressibilities of the oxygen-vacancy-rich perovskites are in agreement with experimental results.

(Philosophical Transactions of the Royal Society of London A360, 2507-2520)
For reprints contact John P. Brodholt: j.brodholt@ucl.ac.uk or Artem R. Oganov: a.oganov@ucl.ac.uk

Magnetic properties of finite Co chains on Pt(111)

B. Lazarovits[1], L. Szunyogh[1,2] and P. Weinberger[1]

[1] *Center for Computational Materials Science, Technical University Vienna, A-1060 Gumpendorferstr. 1.a., Wien, Austria*

[2] *Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521, Budapest, Hungary*

Abstract

We present *first principles* calculations of the magnetic moments and magnetic anisotropy energies of finite monoatomic Co_n ($1 \leq n \leq 10$) chains deposited along the (110) direction on top of a fcc Pt(111) surface. The calculations were performed fully relativistically using the embedded cluster technique within the Korringa–Kohn–Rostoker method. The magnetic anisotropy energy was evaluated by means of the magnetic force theorem. As a direct consequence of the reduced coordination number of the Co atoms, we found enhanced spin- and orbital moments as well as enhanced anisotropy energies in the Co chains as compared to a Co overlayer on Pt (111). For the Pt atoms adjacent to the Co atoms, however, we obtained induced magnetic moments smaller than in the case of a Co monolayer on Pt(111). The moments and the contributions of the individual atoms to the magnetic anisotropy energy depend characteristically on the position within the chains, i.e., on the local environment of the individual atoms. Independent of the length of the chains we found that the easy axis is perpendicular to the surface. The size of the calculated magnetic anisotropy energy and of the anisotropy of the orbital moment fits very well to available experimental values for monoatomic Co chains deposited on a Pt(997) surface.

(Submitted to Phys. Rev. B)

Postscript preprints available from Bence Lazarovits: `bl@cms.tuwien.ac.at`

This paper includes acknowledgement to the RTN on "Computational Magnetoelectronics" (Contract No. HPRN-CT-2000-00143).

The $Pt_{80}Fe_{20}$ surface from first principles: Electronic structure and adsorption of CO and atomic H

Robin Hirschl
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Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria
Françoise Delbecq, Philippe Sautet
Institut de Recherches sur la Catalyse, CNRS, 2 Avenue Albert Einstein, F-69626 Villeurbanne Cedex, and Ecole Normale Supérieure de Lyon, 46 Allée d'Italie, F-69364 Lyon Cedex 07, France
Jürgen Hafner
Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

Abstract

The electronic structure and the local adsorption properties of the $Pt_{80}Fe_{20}$ (111) alloy surface have been theoretically studied in comparison to a pure Pt (111) surface in the framework of spin-density functional theory. Pt-based alloys are important catalysts for the production of unsaturated alcohols. According to several experimental determinations of the surface composition, the surface is modeled by a Pt_3Fe bulk alloy terminated by a single layer of pure Pt . Test adsorbates are CO and atomic hydrogen. Iron atoms bond strongly to neighboring Pt atoms, thereby shifting their d-bands towards higher binding energies and reducing their chemical reactivity. The site dependence of those effects could be resolved by evaluating the partial densities of states of individual d-band orbitals. Though only iron atoms carry a magnetic moment spin polarization is qualitatively important. In a second step we investigated the influence of iron atoms in the surface layer, using Pt_3Fe (111) as a test surface. Here an additional effect of local strain adds to the electronic changes through heteroatomic bonds.

(Phys. Rev. B **66**, 155438 (2002))
Contact person: R. Hirschl (robin.hirschl@univie.ac.at

Ab-initio density functional study of O on the Ag(001) surface

M. Gajdoš, A. Eichler and J. Hafner
Institut für Materialphysik and
Center for Computational Materials Science, Universität Wien,
Sensengasse 8/12, A-1090 Wien, Austria

Abstract

The adsorption of oxygen on the Ag(100) is investigated by means of density functional techniques. Starting from a characterization of the clean silver surfaces oxygen adsorption in several modifications (molecularly, on-surface, sub-surface, Ag_2O) for varying coverage was studied. Besides structural parameters and adsorption energies also work-function changes, vibrational frequencies and core level energies were calculated for a better characterization of the adsorption structures and an easier comparison to the rich experimental data.

(Submitted to Surface Science)
Manuscripts available from: Marek.Gajdos@univie.ac.at

Ab initio calculated electronic structure of metallic nanowires and nanotubes

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Abstract

Ab initio calculations of the electronic structure of freestanding Cu and Na nanowires and nanotubes will be presented. The calculations are based on density functional theory using a Screened Korringa-Kohn-Rostoker method. The nanowires are described by an underlying fcc lattice with a cross section of four to 100 atoms. We assume translational invariance in the direction along the wires. The thickness dependence of the nanowires for the bandstructure and the density of states will be discussed. The electronic structure clearly shows features of the one dimensional system, that is, minibands due to quantum confinement and $1/\sqrt{E}$-singularities in the density of states (DOS). We have analyzed the quantum confinement of the eigenstates. We will discuss the thickness and shape dependence of the subbands and the role of d-electrons by comparing the results of Cu and Na wires.

(Phys. Rev. B, in press)
Manuscripts available from: P.Zahn@physik.tu-dresden.de

Limitations of the two-media approach in calculating magneto–optical properties of layered systems

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Abstract

It is shown that in polar geometry and normal incidence the 2×2 matrix technique – as discussed in detail in a preceding paper [Phys. Rev. B 65, 144448 (2002)] – accounts correctly for multiple reflections and optical interferences, and reduces only in the case of a periodic sequence of identical layers to the Fresnel formula of reflectivity, which in turn is the theoretical basis of the two–media approach, widely used in the literature to compute magneto–optical Kerr spectra. As a numerical example ab–initio calculations of the optical constants for an fcc Pt semi–infinite bulk using the spin–polarized relativistic screened Korringa–Kohn–Rostoker method show very good agreement with experimental data.

(To appear in Phys. Rev. B 66, 1744XX (2002))

Postscript preprints are available from A. Vernes (`av@cms.tuwien.ac.at`)

Broken symmetries in the crystalline and magnetic structures of γ-iron

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Abstract

It is by now well established that in antiferromagnetic γ-Fe, stabilized in the form of precipitates in a Cu matrix or by epitaxial growth on an appropriate substrate, magnetic and/or crystalline symmetries are broken. Little is known, however, on the physical effects driving the symmetry-reduction, and on the interplay of crystalline and magnetic symmetry breaking. We have used a recently developed unconstrained vector-field description of noncollinear magnetism, implemented in an *ab-initio* spin-density-functional code, to search for the magnetic and crystalline structure of γ-Fe, stabilized by different types of constraints. We show that in near face-centered-cubic γ-Fe, stabilized by three-dimensional constraints, the magnetic groundstate is a spin-spiral with propagation vector $\vec{q} = \frac{2\pi}{a} \times (0.2, 0, 1)$ at an equilibrium atomic volume of $\Omega = 10.63$ Å^3, very close to the propagation vector $\vec{q}_{\rm exp} = \frac{2\pi}{a} \times (0.1, 0, 1)$, determined experimentally, but at considerably lower volume than the atomic volume of the γ-Fe precipitates in Cu on which the experiments were performed ($\Omega = 11.44$ Å^3). At these larger volumes our calculations predict an helical spin solution at $\vec{q} = \frac{2\pi}{a} \times (0, 0, 0.6)$ to be the groundstate. Epitaxially stabilized γ-Fe is found to be unstable against both tetragonal distortion as well as monoclinic shear deformation, and the structural distortions suppress the formation of spin-spiral states, in agreement with experimental observations on Fe/Cu(100) films.

(Accepted, Phys. Rev. B)
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Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(001)

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Abstract

Adsorption at surfaces can be modelled using a periodic supercell approach or using finite clusters. For many systems and properties these models are complementary and often the most productive way to work is to use a combination of these techniques. If reliable data is to be obtained it is essential that convergence is achieved with respect to the size of supercell and cluster. This work discusses the convergence of chemisorption properties of H on Cu(001) with respect to the cluster size. To this end calculations of the H binding energy and equilibrium distance, are reported for cluster models of increasing size containing up to 77 metal atoms. Likewise, periodic slab model calculations are used to provide the corresponding values towards which the cluster approach should converge. In many previous studies of a wide variety of systems it has been established that computed equilibrium distances converge rapidly with respect to cluster size. Here, a systematic study of the dependence on cluster size shows that, for adsorption in the 4-fold site, convergence is not achieved even for very large clusters. The reason for this poor convergence is seen to be the inability of the cluster model to reproduce accurately the charge density and electrostatic potential of the crystalline surface

(accepted: Surface Science)

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Surface structure of GaAs(2 5 11)

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Abstract

GaAs samples with orientations vicinal to (2 5 11) within 1° were prepared by molecular beam epitaxy and analyzed in situ by scanning tunneling microscopy, low-energy electron diffraction and reflection high-energy electron diffraction. In addition, first-principles electronic structure calculations were carried out. GaAs(2 5 11) is a stable surface whose orientation is located within the stereographic triangle. For a wide range of As-rich conditions a (1×1) reconstruction forms that is characterized by an inclined series of three As dimers and that fulfills the electron counting rule. The terrace size is limited only by the macroscopic off-orientation of the samples. The surface is perturbed by thin stripes of the nearby orientation (3 7 15). While the dangling bond densities of GaAs(2 5 11) and GaAs(3 7 15) are almost equal, GaAs(3 7 15) violates the electron counting rule. The analysis of this perturbation suggests that, in general, on semiconductor surfaces the gain in stability arising from the minimization of the number of dangling bonds is significantly greater than the gain arising from reaching a semiconducting ground state. Upon annealing of the samples in ultra high vacuum, a fairly rough surface structure develops whose mean orientation is different from (2 5 11).

(submitted to: Phys. Rev. B)
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Comment on "Anomalous Mobility of Strongly Bound Surface Species: Cl on GaAs(001)-$c(8\times2)$"

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Abstract

Although strongly bound chemisorbates at low coverage readily diffuse on metal surfaces at 300 K, they generally do not diffuse on semiconductor surfaces because of a large corrugation in the adsorbate-surface interaction potential. Chlorine chemisorbed on the Ga-rich GaAs(001)-$c(8\times2)$ surface has anomalously fast diffusion even though the chemisorption state is tightly bound and highly specific. The original analysis of the detailed scanning tunneling microscopy (STM) study by McLean *et al.* [Phys. Rev. Lett. **85**, 1488 (2000)] was based on an assumed surface reconstruction that was quantitatively and qualitatively incorrect. Our density-functional-theory calculation of the Cl adsorption and diffusion at the new ζ geometry of the Ga-rich GaAs surface explains the experimental observations.

(Phys. Rev. Lett., in print)
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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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Thermodynamics of the wetting layer in InAs/GaAs(001) heteroepitaxy

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Abstract

The effect of strain and chemical environment on wetting in the initial stages of InAs/GaAs (001) heteroepitaxy are quantifed from first principles. Formation of InGaAs surface alloy is proved favorable for submonolayer InAs coverage under As-rich conditions. Spatially selective wetting on a substrate with inhomogeneous strain distribution is predicted.

(submitted to: Phys. Rev. Lett.)
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Understanding the growth mechanisms of GaAs and InGaAs thin films by employing first-principles calculations

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Abstract

We demonstrate the use of density-functional theory (DFT) calculations for understanding molecular beam epitaxy of GaAs and InGaAs films at the atomic level. For analyzing island growth in homoepitaxy of GaAs(001), the use of DFT in conjunction with kinetic Monte Carlo simulations is discussed. This approach enables us to elucidate the growth mechanisms of islands on the $\beta 2(2\times4)$-reconstructed surface and to compute the saturation values of the island density. Furthermore, DFT calculations are employed to investigate the stability of ultrathin InGaAs films on GaAs(001) as a function both of the chemical potential of arsenic in the growth environment, and of mechanical strain. Under very As-rich conditions, for deposition of two thirds of a monolayer of InAs, our calculations indicate the formation of a (2×3)-reconstructed InGaAs(001) surface alloy. The calculated atomic structure is in excellent agreement with X-ray diffraction data. For less As-rich conditions and larger amounts of deposited InAs, we find InGaAs films with a $\alpha 2(2\times4)$ reconstruction to be most favorable.

(submitted to: Appl. Surf. Sci.)
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9 Book Announcements

P. Mohn, Vienna University of Technology, Vienna, Austria

Magnetism in the Solid State, An Introduction

Approx. 230 pp. 59 illus.

(Springer Series in Solid-State Sciences, Vol. 134)

Hardcover. Approx. EURO 69,95 excl. vat.

Date of publication: November 2002

This book presents a phenomenological approach to the field of solid state magnetism. After introducing the basic concepts from statistical thermodynamics and electronic structure theory, the first part discusses the standard models for localized moments (Weiss, Heisenberg) and delocalized moments (Stoner). This is followed by a chapter about exchange and correlation in metals, again considering the results for the localized and delocalized limit. The book ends with a chapter about spin fluctuations, which are introduced as an alternative to the finite temperature Stoner theory.

Contents: A Historical Introduction.- Consequences of Fermi Statistics.- Paramagnetism.- Energy Bands in the Crystal.- Experimental Basis of Ferro-magnetism.- Weiss Molecular Field Model.- Heisenberg Model.- Itinerant Electrons at 0K.- Band Gap Theory of Strong Ferromagnetism.- Magnetism and the Crystal Structure - Covalent Magnetism.- Magnetic Impurities in an Electron Gas.- Itinerant Electrons at $T > 0$; A Historical Chapter.- Hubbard Model.- Landau Theory for the Stoner Model.- Coupling between Itinerant and Localized Moments.- Origin of the Molecular Field.- Exchange and Correlation in Metals.- Spin Fluctuations.- Single Particle Excitations Versus Spin Waves.- Landau-Ginzburg Model for Spin Fluctuations.- Conclusion and Outlook.- Appendices

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10 Call for Nominations for Michelson Postdoctoral Prize Lectureship

Michelson Postdoctoral Prize Lectureship

Case Western Reserve University

Nomination are invited for the seventh annual Michelson Postdoctoral Prize Lectureship, to be held Spring 2003 in the Dept of Physics, Case Western Reserve University. This prize is awarded annually to a junior postdoctoral scholar active in any field of physics. The winner will spend one week in residence at CWRU and deliver 3 technical lectures and a colloquium. The lectureship carries an honorarium of $1000 plus all travel expenses.

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Deadline for receipt of all materials: Dec 13, 2002.

Pseudo-interactions and the electron-electron cusp

Stephen Fahy, Paul Delaney, and Jim Greer

Department of Physics and NMRC, University College, Cork, Ireland

Abstract

Within this contribution, we discuss a recent study [D. Prendergast, M. Nolan, C. Filippi, S. Fahy and J.C. Greer, Journal of Chemical Physics **115** 1626 (2001)] whereby the electron-electron interaction is replaced by a pseudo-interaction. The pseudo-interaction is chosen to eliminate electron-electron cusps in the many-body wavefunction, and we use this property to study the role of the cusp on convergence in configuration interaction (CI) calculations. Surprisingly, we find that the electron-electron cusp plays little role in determining CI energies, and for chemical accuracy, the slow convergence of CI calculations can not be attributed to fitting electron-electron cusps.

1 Introduction

In this short highlight, we discuss a method of modifying the Coulomb interaction for short electron-electron distances, while maintaining many-body eigenstate energies close to those of the true interaction, which could be expected to improve the convergence properties for configuration interaction (CI) expansions. The method is based on analogous ideas for treating electron-ion interactions with norm-conserving pseudopotentials in order to improve the convergence properties of plane-wave expansions for single-particle wavefunctions. We will show that a representation of the cusps in electronic structure theory turns out *not* to be critical to determination of electronic energies when required to "chemical accuracy" ($\approx$ 1 milliHartree): this result is contrary to commonly held assumptions within the electronic structure community.

The divergence of the $1/r$ electron-electron interaction in many-electron systems (all quantities in atomic units) produces an infinite potential energy at electron-electron coalescences. However, since an eigenstate ψ of the Hamiltonian H, with energy E, satisfies the Schrödinger equation, $H\psi = E\psi$, the local energy $(H\psi)/\psi = E$ at such coalescences does not diverge. This non-divergent local energy is guaranteed by the imposition of cusp conditions on the many-body wave function [1] where two electrons coincide, causing the infinite potential energy to be cancelled

by an equal and opposite divergence of the kinetic energy (the same phenomenon occurs for electron-nucleus interactions).

Configuration interaction calculations use an expansion in configuration state functions comprised of spin coupled sums of determinants built from single-particle orbitals. It has been stated that the expansion is slowly convergent because, being a smooth function of the separation between any two electrons, it cannot easily reproduce the required cusps in the wavefunction at electron-electron coalescences [2]. To avoid this difficulty, we replaced the divergent $1/r$ electron-electron interaction with an interaction that is smooth and finite at the origin [3]. Much to our surprise, we found this removal of the cusp made little difference to the convergence of CI expansions at the approximation level of a milliHartree per atom.

In the approach outlined here, we show how to keep the energy and the intermediate- and long-range correlation properties of the many-body eigenstate unchanged. In particular, our new (smooth) interaction should ideally have scattering properties identical to the true interaction for all energies. If this were the case, all many-electron eigenvalues would be identical for both interactions. While this is the ideal, we expect that a potential which gives the same scattering properties as the true interaction over a sufficiently wide range of scattering energies will give many-electron eigenvalues very close to the true interaction.

This problem (for electron-electron scattering) is analogous to the problem of electron-ion scattering addressed in the pseudopotential method. In that approach, the aim is to produce a smooth electron-ion potential which reproduces the single-particle eigenvalues of the true system over a range of energies, and has the same single-particle wavefunctions outside some suitably chosen cut-off radius. Such pseudopotentials are generated for the isolated atom but may then be used with a high level of accuracy in molecules and solids

Following the success of norm-conserving pseudopotential methods in the context of the electron-ion scattering problem, we generate from consideration of the two-electron scattering problem a norm-conserving pseudo-interaction which is intended to replace the true $1/r$ electron-electron interaction. This is presented in Section 2 of the paper. Since the electron-electron interaction is repulsive and has no bound states for an isolated pair of electrons, we use, with some minor modifications, the generalized norm-conserving method devised by Hamann [4] to generate pseudopotentials for electron-ion interactions at unbound, scattering state energies. In section 3, discussion of the method for configuration interaction methods is presented. We indicate how standard algorithms for the calculation of two-electron integrals in a Gaussian expansion can be modified for our pseudo-interaction. We have demonstrated the application of the pseudo-interaction to dynamical CI methods whereby configuration state functions are not selected *a priori*, but are included based upon a selection criterion as the calculation proceeds. Hence methods with a predefined number of configurations such as singles and doubles CI, or other excitation truncated methods, are not pertinent to our discussions, but methods such as a Monte-Carlo generation of configurations (MCCI) [5, 6] and the use of a second-order perturbation scheme for the selection of configurations [7] are well-suited to a pseudo-interaction approach. We will find however, that the CI expansions actually introduce very few functions for fitting the cusps for accuracies typically required — hence the belief that the obstacle to convergence in CI calculations is due to fitting the cusps has been found to be *untrue* for calculations

of chemical accuracy.

2 Construction of generalised norm-conserving pseudopotentials for electron-electron interactions

This procedure follows that set out by Hamann [4] for producing generalised norm-conserving pseudopotentials (GNCPP's), with relatively minor modifications. There are two differences between our electron-electron scattering problem and the electron-ion pseudopotential generation treated by Hamann: (i) Only two particles are involved in the generation of the electron-electron pseudo-interaction, so that we do not need to include screening potentials; (ii) because we are solving the scattering problem in the centre of mass frame of the electrons and use the relative coordinate $\mathbf{r}$ of the electrons, the mass of the electron is replaced by the reduced mass for the two-electron system. Using Hartree atomic units throughout, the interaction potential is then $V(r) = 1/r$ and the reduced mass is $1/2$. The absence of screening simplifies some of the steps laid out in Hamann's work. Full technical details of how to generate the pseudo-interaction are given in Ref. [3] and we only briefly discuss some qualitative issues here.

2.1 Two-electron Scattering

The radial Schrödinger equation for the relative motion of two electrons is

$$-\frac{d^2u_l}{dr^2} + \left(\frac{l(l+1)}{r^2} + (V-\epsilon)\right) u_l = 0, \tag{1}$$

where $u_l(r)$ is r times the wave function in the relative coordinates, with angular momentum l and energy ϵ. In the norm-conserving pseudopotential approach, different scattering potentials are often generated for different values of the angular momentum l. The full many-body wavefunction is anti-symmetric with respect to exchange of any two electrons. Thus, if the spins of the two electrons are parallel, the orbital part of the wave function must have odd parity in their relative separation and the allowed angular momentum l in Eqn. (1) must be odd. The dominant parallel-spin scattering would then have $l = 1$. For singlet (anti-parallel) scattering, the spin part of the two-electron wavefunction is anti-symmetric, so that the orbital part is symmetric and l must be even. In this case the dominant allowed angular momentum is $l = 0$.

Following the usual pseudopotential approach, we might then expect to generate a parallel-spin scattering potential using $l = 1$ and an anti-parallel-spin scattering potential using $l = 0$. In practice, we find that the $l = 0$ potential gives good scattering for both angular momenta and the use of separate parallel- and anti-parallel-spin potentials is unnecessary.

The eigenvalue ϵ is the kinetic energy of the electrons in the centre of mass frame. In the generation of a pseudopotential, the real potential and pseudopotential become identical outside a suitably chosen cut-off radius r_c and are constructed to have identical scattering phase shifts and energy derivative of the phase shift at a reference energy. The choice of ϵ_l is important for large values of the cut-off radius. However, for values of the cut-off radius which one would expect to use in a calculation the choice of ϵ_l is not expected to be crucial.

The choice of an appropriate cut-off radius r_c is determined by the properties of the system in which we plan to use the pseudo-interaction. If r_c is chosen to be extremely small, then the interaction is almost numerically identical to the true interaction. At the other extreme, if the cut-off radius is chosen to be much larger than the system size, the electron-electron interaction will hardly depend at all on the distance between the electrons and we will obtain essentially the properties of a non-interacting system.

In the generation of norm-conserving pseudopotentials for electron-ion interactions, it is generally found that the maximum cut-off radius for accurate transferable pseudopotentials is approximately half the radius at which $u_l(r)$ of the relevant valence state has its outer-most maximum. This forces the pseudo-wave-function to converge to the full-potential wave function somewhat inside this maximum, which typically occurs near the relevant radius for bonding in such states. We found that a similar criterion, applied to the electron pair distribution function, determines the maximum cut-off radius for highly accurate electron-electron pseudo-interactions.

3 CI Convergence and Implementation of The Pseudo-Interactions

3.1 CI Calculations and Pseudointeractions

Although the CI method can give an exact solution of the Schrödinger equation in a finite basis set, it requires an extremely large number of configuration state functions (CSFs), and hence extremely large vector and matrix dimensions. It is generally accepted that the slow convergence of the CI expansion is partly due to the electron-electron cusp, as discussed earlier in this paper. It has been demonstrated, both theoretically and numerically, that the convergence of a CI calculation, using Slater determinants built up from single-particle functions, is proportional to l^{-3}, where l is the maximum angular momentum in the basis set. Explicit inclusion of terms in the inter-electronic distance as in Hylleraas' He work [8], the more modern work of Kutzelnigg and Klopper [9], or the use of explicitly correlated (geminal) Gaussian basis functions [10], can improve the convergence of a CI calculation and the calculation can be found to converge as l^{-6} or better [11]. The accepted reason for the success of methods which explicitly include r_{12} is that they give a correct description of the short-range part of the interaction. Baker *et al* [12] also showed that using basis functions with the same analytic structure as the function one is trying to fit (inclusion of powers of r_{12} and logarithmic terms in r_{12}) can lead to a reduced expansion length, a technique pioneered by Pekeris [13]. However, these methods are outside the mainstream of quantum chemistry, and can not easily avail of the standard numerical tools applied within such calculations, or are only applicable to two electron problems.

An electron-electron interaction potential which is smooth at short-range and finite at the origin will have smooth electron-electron coalescences. Hence it has been generally accepted that pseudo-interactions which are finite at the origin would be expected to give better convergence in terms of the number of expansion functions required to provide a given accuracy in the energy [9, 11, 14, 15, 16], as compared to a pure Coulomb interaction. Although this point had been stated in the literature, there appear to be no numerical expositions of this prior to the numerical study of Prendergast *et al.*[3]. As far as we are aware, this was the first time that the actual convergence of a CI expansion had been examined in the case where the electron-electron

interaction is given by a function which does not contain an electron-electron cusp.

3.2 Evaluation of Two-Electron Gaussian Integrals with Pseudo-Interactions

The implementation of the scattering potential in CI calculations involves fitting the numerically generated pseudo-interaction to a sum of terms which can be evaluated analytically in the Gaussian CI basis functions, as follows:

$$V_{ee} = \mathrm{erf}\frac{(\mu r)}{r} + \sum_{i=1}^{n_G} c_i \exp(-a_i r^2) \tag{2}$$

Rys quadrature [17] is a standard numerical scheme for the calculation of two-electron Coulomb integrals in a Gaussian basis. The details, such as the calculation of the the number of quadrature roots, their values and weights, as well as the motivation for the Rys quadrature method may be found in the paper by Dupuis, Rys and King [17], and references therein. Details of how to simply modify the Rys quadrature approach to calculate two-electron intergrals for an interaction represented by Eq. (2) are given in Ref. [3]. We have applied the modifications to the calculation of two electron integrals within the ARGOS code, part of the COLUMBUS program package [18].

4 Results and Conclusions

We have applied the pseudo-interaction method to the calculation of correlated atomic energies for helium and beryllium using a sequence of basis functions including up to g functions. As we have described, we have employed the MCCI method for calculation of electronic energies. This is an important feature of our study as the MCCI method is not an excitation truncated method, *i.e.* the number of CSFs to include in a calculation is not *a priori* fixed. Rather, the MCCI method randomly selects CSFs, retains important configurations, and iterates this procedure until the energy (and number of CSFs) converges.

Let us consider what this implies for calculations using the electron-electron pseudo-interaction. When the MCCI method converges, it has a set of CSFs which best represent the total correlation energy for a given CI vector coefficient threshold. Hence the CI vector is the set of "best" CSFs to describe to correlation energy, and based upon exact studies of fitting the correlation cusp using higher angular momentum functions, we would anticipate the CI vector will increase in length as higher angular momentum functions are included into the basis, and that these are included into the calculation primarily by the need to better describe the electron-electron cusps.

We now turn on the pseudo-interaction, and increase the cut-off radius and eliminate the cusps. We would then anticipate that the number of CSFs needed to describe the cusp region is decreased, and that this achieved at little cost to the accuracy in the total energies. Hence, when the MCCI calculation converges with pseudo-interaction replacing the true Coulomb interaction, we would expect to converge to a CI vector with the number of "best" CSFs substantially less than for the full interaction Hamiltonian.

Returning to our numerical studies where we have studied the convergence properties of CI calculations as function of CI vector coefficient threshold, pseudo-interaction cut-off radius, and

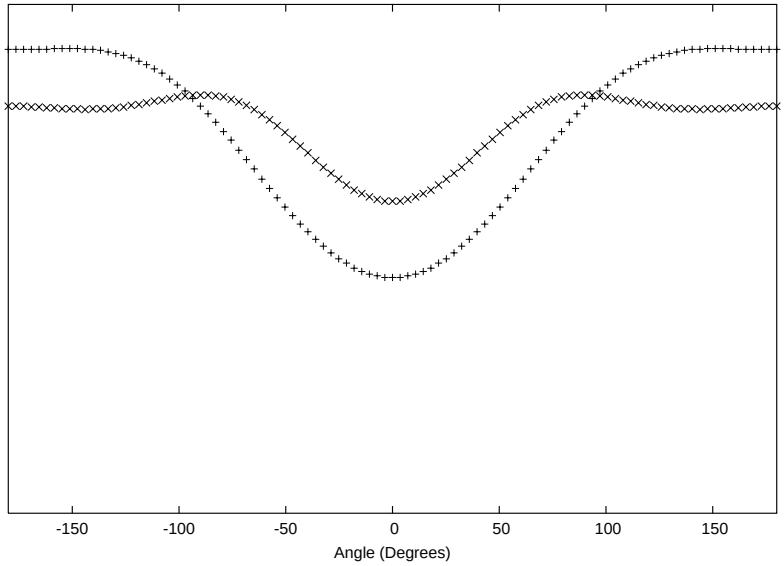

Figure 1: The two-body reduced density matrix calculated for atomic helim calculated using the cc-pvDZ (x) and cc-pvQZ (+) basis sets (vertical axis in arbitray units). The increase in the number of basis functions and in particular the increase in angular momentum in going to the larger basis set improves the description of the cusp region. However, smoothing the cusps does not reduce the effort needed to describe the correlation hole.

angular momentum in the single particle basis expansion [3]. The calculations were performed for He and Be. Without overly belaboring the point, we found that replacement of the pseudo-interaction *did not* significantly reduce the number of CSFs needed to describe the correlated systems (readers seeking the explicit details are referred to ref. [3]). The assumption that the additional CSFs needed in a CI expansion to converge to the full CI (FCI) energy are needed primarily to describe the cusp region is incorrect. This is our primary conclusion.

We now seek to reconcile this result with properties known for treating the cusp. For example, in ref. [19] the asymptotic form of wavefunction as a function of angular momentum is derived for the helium cusp. In the asymptotic regime, higher angular momentum functions ($l > 30$) are required to achieve microHartree accuracy in the total energy. Here we are working to chemical accuracy (milliHartree) and the maximum angular momentum function considered is g ($l = 4$). We have fitted the convergence of the total energy to the asymptotic form and find that, although the general behaviour of the asymptotic form is observed, the coefficients extracted are not equivalent to the asymptotic coefficients. Hence we are not working in the asymptotic region and the requirements to describe the cusp region to chemical accuracy are significantly less demanding. In fig. 1, we plot the the two-body reduced density function $\Gamma(r_1; r_2)$ for atomic helium with one electron fixed at a distance of 0.5 a.u. from the nucleus, and the second electron is allowed to move on a circle of radius of 0.5 a.u. The electron cusp occurs when the two electrons coincide, and as expected, the CI wavefunction improves at the cusp as the basis is increasd. However, even for larger values of angular momentum typically used in CI calculations, the cusp region is not particularly well-described. Smoothing the cusp does not reduce the number of configurations required to describe the vicinity of the electron, and a more accurate representation of the cusp regions does not provide a significant improvement in the

electronic energy.

Finally, we point out that the results of our study are consistent with arguments put forward by Gilbert [20], who in 1963 anticipated the results of our detailed numerical study. Gilbert argued that the cusp region was not the limiting factor for an accurate treatment of the correlation energy, but that intermediate range correlations (i.e. for typical electron-electron separations) are the practical limiting factor to convergence in CI calculations. He argued that the contribution to correlation energy from a poor representation of the cusp is relatively small, and that the use of basis functions relative to a fixed spatial reference were unable to easily treat correlations for typical inter-electron separations. After nearly 40 years, we can now substantiate his considerations.

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