Ψ_k Newsletter

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

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1 Editorial

We would like to turn our readers attention to the **General News** section where we call for ideas on how to make our next newsletter, the 50th issue, a special one. There we also ask for submissions of abstracts and applications for collaborative visits. The **News from the RTN** section is particularly bulky, since we have there a report on the first year activity of this network plus a detailed report on its First Annual Meeting in Budapest last September, including abstracts of presented papers. In this newsletter we also have some news from the TMR2 Network and write about two new RTN networks, within the Fifth Framework, in the field of ab-initio calculations, whose contracts are being currently negotiated with the EU in Brussels. In the **News from the ESF Programme** section we have two conference announcements. Three more conference/workshop announcements can be found in the **General Workshop/Conference Announcements** section. A number of available positions are announced in the usual **General Job Announcements** section. Abstracts of recent or newly submitted papers are in the Abstracts section, which is followed by the announcement of a Car-Parrinello Molecular Dynamics Program, developed by the Stuttgart group with J. Hutter, M. Parrinello, and others. The newsletter is finished with the scientific highlight by Michael Springborg, Jan-Ole Joswig, Valeri G. Grigoryan, Christian Gräf, Sudip Roy, and Pranab Sarkar *Physical Chemistry, University of Saarland* on **"Optimizing Structure for Larger, Finite Systems"**. 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
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2 General News

2.1 Call for Special Submissions to the 50th Psi-k Newsletter, Abstracts of Newly Submitted Papers, and Applications for Collaborative Visits

Note that the next Psi-k Newsletter, the April issue, will be our jubilee, 50th, issue and we would like to make it a little bit more special. Therefore, we would like to invite all our readers to submit to us their ideas on how to make this special issue more rewarding to all. If you have any contributions in mind that would make the April newsletter special, we would like to hear from you as soon as possible. We have only two months for preparing the next Psi-k Newsletter and therefore would appreciate very much your full cooperation and support.

Recently 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 you all to send us your abstracts. The abstract template is available in every LaTeX file of the Psi-k newsletter. If you feel however that it takes too much of your effort, 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.

We would like to remind our readers that the current year is the last year of the ESF Programme activity. The Programme still has at its disposal money for collaborative visits and secondments. Therefore we would like to encourage all the members of the Psi-k community, originating from the 17 member countries participating into the Programme to make use of this opportunity. One just needs to submit a one page proposal to the Core Steering Committee of the ESF Programme (psik-management@dl.ac.uk), stating the purpose of the visit and describing briefly the project as well as the financial support being sought. The Core Steering Committee of the ESF Programme can make a quick decision after consultations by email. The countries contributing to the ESF Psi-k Programme are: Austria, Belgium, Czech Republic, Denmark, Finland, France, Germany, Hungary, Ireland, Italy, Poland, Portugal, Slovenia, Spain, Sweden, Switzerland, and the United Kingdom. Please check http://psi-k.dl.ac.uk for further details on how to make a collaborative visit.

3 News from the Research Training Network (RTN)

COMPUTATIONAL MAGNETOELECTRONICS

3.1 First Annual Report on the Network's Activity

Research Objectives

Magnetoelectronics means, in the broadest possible terms, the manipulation of the electronic charge transport by the spin-degrees of freedom. In the more narrow technical sense it refers to a new electronics which uses magnetoresistive properties in device applications.

The aim of the present network on "Computational Magnetoelectronics" is to use the power of Density Functional Theory (DFT) to model, understand and predict the transport properties of materials and material systems relevant to magnetoelectronics. This is a very focused effort of leading European computational groups. It aims at the calculation of electronic states at, and spin-dependent transport through, interfaces, junctions and other two dimensional nanostructures of relevance to magnetoelectronics. Most of the calculations are based on DFT in the local density approximations (LDA) or the generalised gradient approximation (GGA). However, where necessary, more sophisticated methods like the GW approximation, LDA+U, SIC, screened exchange and dynamical mean field are being deployed. The usefulness of this methodology has expanded enormously since the first applications some 25 years ago: an increase of approximately a million times in computer power, the development of new conceptual tools like Green's functions and screening, the accuracy of the local density approximation, all contributed to its huge success. The reliability of these Density Functional Theory calculations is such that they can guide experiments in detail and even substitute for them. This new role of theory is well characterised by the fact, that in the last years several groups in this Network (Twente, Juelich, and Uppsala) have obtained patents in the field of magnetic multilayers solely based on computational studies. The calculations are performed on systems of relevance to technology and industry guaranteed through the participation of the industrial partner Thomson as a subnode and close interactions with Philips and Siemens. Also, the participation of the discoverers of GMR and interlayer coupling strengthens the collaboration with European experimental groups. Moreover, the participation of a US node, unfunded, gives the network access to the latest technological developments in the US.

The research project of the network concentrates on ten flagship projects centered around hybrid interfaces with ferromagnets (FM) and around magnetic nanostructures:

- Interface FM / Semiconductor
- Interface FM / Oxide

- Interface FM / Superconductor
- Magnetic Nanostructures
- Magnetooptics
- Magnetic X-ray Scattering
- Giant Magnetoresistance
- Tunneling Magnetoresistance
- Spintronics
- Experimental Data and Assessement of Applicability

Scientific Highlights

"Large magnetoresistance in Fe/MgO/FeCo(001) epitaxial tunnel junctions", M. Bowen, V. Cros, F. Petroff, and A. Fert

The magnetoresistance of magnetic tunnel junctions (MTJs) is of uncontested interest for important applications with, in particular, promising perspectives for the fabrication of nonvolatile memories (MagneticRAM). Up to now, most studies have been performed on MTJs with a layer of amorphous alumina as insulating barrier between the ferromagnetic electrodes, yielding large and reproducible tunneling magnetoresistance (TMR). However, from a fundamental point of view, i.e., the understanding of the physics of spin-dependent tunneling, a transport study through an amorphous insulator is hardly accessible in a theoretical approach. Most numerical calculations of spin-dependent tunneling and TMR have been developed for single crystal MTJs such as Co/Al2O3/Co(100), Fe/ZnSe(100) or Fe/MgO(100). All emphasize that a correct depiction of the spin-dependent tunneling properties of epitaxial MTJs must transcend the simple potential barrier picture and take into account the interplay of electronic structure between metal and insulator. A test of these models can be performed on single-crystal epitaxially grown structures. Towards this end, M. Bowen, V. Cros, F. Petroff and A. Fert of the experimental Orsay node of the network, in collaboration with A. Cebollada et al. at the IMM-CSIC in Madrid, have obtained the first experimental results showing large TMR values in Fe(001)/MgO(001)/FeCo(001) fully epitaxial tunnel junctions (Appl. Phys. Lett. 79, 1655 (2001)). Tunnel magnetoresistance measurements give 60 % at T=30 K, to be compared with 13 % obtained recently on (001)-oriented Fe/amorphous-Al2O3/FeCo tunnel junctions (Yuasa et al, Europhys. Lett. **52**, 344 (2000)). This difference demonstrates that the spin polarization of tunneling electrons is not directly related to the density of states of the free metal surface - Fe (001) in this case - but depends on the actual electronic structure of the entire electrode/barrier system.

"Spin-polarized current induced switching", Peter M. Levy, Shufeng Zhang, Albert Fert

The concept of switching the orientation of a magnetic layer of a multilayered structure by the current perpendicular to the layers was introduced by Slonczewski and Berger. The central idea is that for a noncollinear configuration of the moments of the magnetic layer the current induces a torque acting on the spins of the conduction electrons which in turn transmit this torque to the background magnetization of the magnetic layers through the exchange interaction between

conduction electrons and the local "d" electrons. An alternate mechanism of current induced switching was put forth by Heide in which the current across the magnetically inhomogeneous multilayer produces spin accumulation which establishes an energy preference for a parallel or antiparallel alignment of the moments of the magnetic layers; this magnetic "coupling" was posited to produce switching. Recent experiments have reliably demonstrated that the magnetization of a magnetic layered structure is indeed switched back and forth by an applied current. However, it is unclear whether the magnetization switching is triggered by the current-driven effective field or by the spin torque mechanism or both. We have examined the two views of current induced switching, spin torque and effective field, by solving the equations of motion for the spin accumulation and the local magnetization. We find the two mechanisms do coexist; albeit in form different from that originally envisaged. The salient difference between our treatment of spin diffusion and previous treatments, lies in the inclusion of the exchange interaction between the spin accumulation and the magnetic background. With our results, we can understand these two mechanisms on an equal footing: both are simultaneously derived and both depend on the same set of parameters used for understanding the giant magnetoresistance when the current is perpendicular to the plane of the layers (CPP). Furthermore, we have introduced a new length scale for the transverse spin accumulation and clarified the ferromagnetic layer thickness dependence of the switching dynamics. Our solution differs in two important aspects from previous work: we find the longitudinal spin accumulation does not play a role in the switching, and the spin torque and the effective field arises from a region in the magnetic layer within 2-4 nm of the interface. The decay length in our theory is related neither to the phase of the wavefunction, nor to the spin diffusion length as in the effective field concept of switching.

"GMR from first-principle", V. Drchal, J. Kudrnovsky, I. Turek, P. Bruno, P. H. Dederichs, and P. Weinberger

We have developed a versatile and accurate method allowing to investigate from first-principles the spin-dependent conductance in layered systems both in the ballistic and diffusive regimes. We employ the Landauer-type formulation of the transport formulated in terms of the surface Green function approach which is capable to describe the details of the electronic structure of the system both at and/or far from the sample interfaces by treating the sample and the electrodes on the same footing. The substitutional disorder in the sample can be represented by finite two-dimensional supercells each of them containing lattice sites occupied randomly by atoms of (two) different types while electrodes remain non-random. In this way both ballistic and diffusive transport across the multilayer can be treated on equal footing. Finally, non-collinear alignments of magnetizations in different layers, e.g. like in domain-walls and/or in samples with different coercitivities subjected to an external magnetic field can be also treated in the present formalism (spin is then no longer a good quantum number). The theoretical approach was illustrated on disordered fcc(001) spin-valve system with a random CuNi-spacer sandwiched by two ideal Cu leads. The main conclusions of our study can be summarized as follows: (i) The residual resistivity of the disordered alloy forming sample as well as interface resistances (estimated from the slope of the thickness dependence of the resistance and its offset, respectively) agree quantitatively well with experiment as well as with other calculations ; (ii) We have calculated separately the ballistic and diffusive (coherent and incoherent) parts of the

transport and found that within a Landauer-type description of the transport a correct treatment of vertex-corrections is mandatory. (iii) The two-current series-resistor model, widely used for interpretation of experimental result, is valid only for large spacer thicknesses and non-negligible deviations appear for thicknesses comparable to the mean-free path. In particular, the transport may depend on the order of layers in the system (interleaved and separated multilayers); (iv) The finite size of supercells used in calculations leads to some inaccuracies but reasonable results can be obtained for supercells containing already 30-50 atoms which, in turn, allows to treat on first-principle level transport properties of samples containing many hundreds of layers; (v) The GMR ratio is predominantly determined by intrinsic, band-structure effects while the effect of disorder in the sample and/or at interfaces is relatively weak. The approach described here is also suitable for investigating the tunneling magnetoresistance (TMR) of a magnetic tunnel junction.

Additional Research Objectives

In addition to the original research objectives stated above, the Network has decided to introduce a new flagship project "Novel Magnetoelectronics Materials". Since the submission of the application for the RT-Network "Computational Magnetoelectronics", the new field of Magnetoelectronics has progressed enormously. Quite new materials have come into the focus of interest, in particular, correlated systems like transistion metal oxides, perovskites and halfmetallic systems. In addition a strong emphasis is now put on spin-dependent transport in semiconductors, which in particular requires the investigation of magnetic semiconductors and the spin injection from ferromagnets into semiconductors. These new activities are extremely promissing from a scientific as well as technological point of view as has been shown in recent conferences, in particular the "Symposium of Spin-Electronics" in Halle, organized by our Network-member Patrick Bruno. Also in several countries new government projects have been started, e.g. in the USA the new DARPA project "SpinS" (i.e. Spins in Semiconductors).

In the new project "Novel Magnetoelectronics Materials" more emphasis is put on methods which allow to describe correlated electron systems. These are eg. the LDA+U method and the SIC method. In addition, also more demanding methods like the GW approximation and the dynamical mean field approximation are being developed and will be used in the future for these materials.

New tasks have been introduced:

- experimental investigation of magnetization reversal by spin injection in connection with the theoretical models developed in the F-node and US-node collaboration;

- experimental investigation of new half metallic oxydes (such as double perovskites like Sr2FeMoO6 we started to work on during Year 1). These materials have significantly higher Curie temperatures than the $La_{0.7}Sr_{0.3}MnO_3$ compound;

- experimental investigation of magnetic semiconductors such as TM-doped ZnO which are promising for spintronics devices.

A further motivation for introducing the project on "Novel Magnetoelectronics Materials" arises from the cooperation with our industrial/experimental partner Prof. Albert Fert in Paris, who is one of the leading international players in this field. This node needs good theoretical support

to understand their recent experimental results in the electronic properties of these materials. Our Network has world class experience and expertise in studying correlated transition metal oxides such as Sr2FeMoO6 from the Dutch node (Prof. Sasha Liechtenstein) and the UK node (Prof. Walter Temmerman). As a matter of fact, the Daresbury group is already performing calculations for the French node.

Joint Publications and Patents

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55) M. Woods, A. Ernst, P. Strange and W. M. Temmerman,
"Ab initio relativistic spin-polarized theory of angle-resolved photoemission",
J. Phys.: Condens. Matter 13, 8607-8624 (2001) D and UK collaboration.

56) M. Woods, P. Strange, A. Ernst, and W. M. Temmerman,
"First principles relativistic theory of photoemission from magnetic surfaces",
J. Magn. Magn. Mater. 226 - 230,1032 - 1034 (2001) D and UK collaboration.

57) M. Pajda, J. Kudrnovsk, I. Turek, V. Drchal, and P. Bruno,

"Ab initio calculations of exchange interactions, spin-wave stiffness constants, and Curie temperatures of Fe, Co, and Ni",
Phys. Rev. B 64, 174402 (9 pages) (2001) D and CZ collaboration.

58) J. Kudrnovský, V. Drchal, I. Turek, P. Streda, P. Bruno,
"Magnetoresistance in domain walls: effect of randomness",
Surface Science 482 - 485, 1107 - 1112 (2001) D and CZ collaboration.

Organisation and Management

The network's scientific tasks are organised into flagship projects and managed through a board of two to three of the most senior researchers in each node, coordinated through a Chairman and the Network coordinator. An open meeting of this board took place during the Network's annual meeting in Budapest. This meeting reviewed progress so far and in particular concerning recruitement of young researchers.

The network uses the psi-k mailing list- which contains in excess of 900 e-mail addresses of researchers active in ab initio electronic structure calculations to announce its meetings. Reports on these meetings are published in the Psi-k newsletter which is distributed over the same mailing list. This newsletter is published every 2 months and available on the web (http://psi-k.dl.ac.uk). This web page also contains a pointer to the homepage of this RTN.

Report on Network Meetings

The Network organised in its first year three Network meetings, which are reported below. The program of these meetings and the abstracts of all papers can be found in the Psi-k newsletters No 43 (February 2001), No 46 (August 2001) and the present newsletter, respectively. These are available on http://psi-k.dl.ac.uk/psi-k/newsletters.html.

1. RTN Workshop on TMR and GMR in Dresden, Dec. 1 - Dec. 3, 2000

The first workshop of our Network was organised by Ingrid Mertig in Dresden, in the building of the Max Planck Institute "Physics of Complex Systems". It was attended by 54 participants from all nodes of the Network. In addition we had invited several well-known experts (E. Tsymbal, Oxford; J. Barnas, Poznań; G. Mathon, London; G. Schmidt, Würzburg; W. Wulfhekel, Halle, and A. Vedyaev, Strasbourg) to inform us about their recent work. The expenses of these guests as well as part of the expenses of the whole workshop were sponsored by the Max Planck Institute and by the Sonderforschungsbereich 422 of the Technical University Dresden. The workshop consisted of a good mixture of invited reviews and of many contributed papers, presented by the young researchers of our Network. It showed, that all nodes of the Network had already strong activities in Magnetoelectronics. The workshop was accompanied by a management meeting and a general discussion about the future research topics. It was univocally decided that the Network should introduce a new flagship project "Novel Magnetoelectronic Materials".

2. Summerschool on Physics of Magnetic Multilayers in Prag, June 9 - 16, 2001

The European Graduate School on Condensed Matter (EGSCM'01) on the subject "Physics of Magnetic Multilayers - Theory and Experiments" was held in Prague at the Charles University from June 6 - 16, 2001. It was organised by our Czech partners Vaclav Drchal, Josef Kudrnovsky, Ilja Turek from the Academy of Science and by Vladimir Sechovský from Charles University and was jointly sponsored by the ESF-Psi-k Programme and our Network. Most remarkable was the attendance of 113 young researchers, coming from 23 different countries all over the world! The lectures were given by 29 invited speakers, of which about 2/3 were members of our Network. The school consisted of 6 hours of lecture each day, and in addition of two poster sessions, where the young participants could present their work. This school was a huge success, to which, in addition to the excellent program and the good organisation, also the beautiful city of Prague strongly contributed.

3. 1st Annual Meeting in Budapest, Sept. 27 - 30, 2001

The 1st Annual Meeting of our Network was organised by our Hungarian partners János Kollár and László Szungyogh in Budapest, in the Hotel Agro in the Buda Hills. It was attended by 77 participants from all nodes of the Network. The program consisted of 49 short contributions of 15 min each, given mostly by our young students. In addition we had asked six prominent scientists to give reviews on different hot topics in magnetoelectronics. Three of these invited speakers (W.H. Butler from Oak Ridge, USA; H. Katayama-Yoshida from Osaka, Japan; A. Georges from Paris) are leading researchers, not belonging to the Network. In total a huge number of exciting contributions were presented, covering the field of Magnetoelectronics in its whole breath. See the next subsection for further details and the abstracts of presented papers.

During the Management Board Meeting and the Open Discussion the planned Workshop program for the next year was discussed (a Hands-on-Course on Spectroscopy in Munich, a Winterschool on Magnetism in Sweden, a Workshop on Hybride Interfaces in Daresbury and the Annual Meeting in France). It was decided, that due to the large number of contributed papers the next Annual Meeting should also include a poster session.

Networking

Regular e-discussions between all nodes have taken place, leading to 58 common publications.

- Professor P. Weinberger from the A-node has spent a sabatical leave at the Laboratoire de Physique des Solides of Universite Paris-Sud-Orsay (France) from october 1 to december 31, 2000.

- Professor P. Levy from the US-node is presently on sabatical leave from NYU and will be at the Universite Paris-Sud-Orsay (France) until september 2002.

- Dr C. Sommers has visited the A-node from the 25th to the 30th august 2001.

- Dr C. Sommers has participated to the MMM 2001 conference in Seattle, USA

- Several members (C. Sommers, F. Petroff, A. Fert, and others) of the F-node have participated to the MML'01 conference (June 24-29, 2001 in Aachen, Germany). A. Fert had an invited conference paper.

- Nine members of the F-node (among whom 4 resident young researchers) have participated to the 1st Annual Meeting of the network in Budapest.

- I. Turek (CZ) visited P. Weinberger (A) (30 January 2001).

- V. Drchal (CZ) visited P. Weinberger (A) (March-April 2001).

- J. Kudrnovsky (CZ) visited P. Bruno (D-2) (3 months in 2001).

- S. Pick (CZ) visited H. Dreysse (F) (13-26 May 2001).

- I. Turek and J. Kudrnovsky (CZ) visited P.H. Dederichs and S. Blugel (D-1) (24 June - 7 July 2001).

- J. Kudrnovsky and F. Maca (CZ) visited P.Weinberger and J. Redinger (A) (October-November 2001).

- O. Sipr (CZ) visited H. Ebert (D-1) (29 October - 9 November 2001).

- V. Drchal (Prague) visited Juelich, 12-16 Nov. 2000.

- H. Ebert (Munich) visited Warwick, 28-30 March 2001.

- Z. Szotek (Daresbury) visited Juelich, 21 June-17 Aug. 2001.

- W. M. Temmerman visited Juelich, 21 June-17 Aug. 2001.

- S. Bluegel, P. H. Dederichs (Juelich) and H. Ebert (Munich) visit Prague, 8-16 July, 2001.

- P. H. Dederichs (Juelich) visited Dresden, 7-9 July 2001, and Halle, 10-11 July 2001.

- M. Alouani (Strasbourg) visited Juelich, 13-18 Aug. 2001.

- S. Di Napoli (Strasbourg) visited Juelich, 13-26 Aug. 2001.

- L. Udvardi (HU) visited Vienna April-June 2001.

- J. Kollar (HU) visited Uppsala for one week February 2001.

- K. Palotas (HU) participates in the Prague summerschool.

- B. Magyari-Kope (HU) attends a Conference in Madrid.

- 2-month visit of Peter Mohn (TU Wien) in Uppsala (October/November 2000).

- 2-month visit of Liviu Chioncel (Katholieke Universiteit Nijmegen, The Netherlands) in Uppsala (1/3-1/5 2001).

- 1-week visit of Peter Zahn (Dresden) in Uppsala (September 2001).

- W.M. Temmerman and Z. Szotek (Daresbury) visit Halle (summer 2001).

- A. Ernst and D. Koedderitzsch (Halle) visit Daresbury Laboratory (November 2000).

- B.L. Gyorffy (Bristol) visited Halle (January 2001).

- O. Bengone (Uppsala) visited Strasbourg 1-11 June 2001.

- S. Lebeque (Strasbourg) visited Juelich 13-19 August 2001.

- G. Heisnen (Nijmegen) visited Strasbourg 20-25 August 2001.

Training of young researchers

The Network's young researchers attended the Dresden workshop, Prague Summer School, Budapest Annual Meeting, and the Spin Electronic Symposium in Halle. In particular, the UK, German, Austrian and Dutch young researchers attended the Prague summer school, the Dutch and Austrian young researchers attended the Dresden workshop and all young researchers attended the annual meeting in Budapest. Additionally, the Swedish young researcher (Oliver Bengone) spend two weeks in the French node in Strasbourg .

3.2 Reports on RTN Workshops and Meetings

3.2.1 Report on the First RTN Annual Meeting

1st Annual Meeting
of the Research Training Network
Computational Magnetoelectronics

September 27-30, 2001, Budapest, Hungary

The first Annual Meeting of the Research Training Network "Computational Magnetoelectronics" was organized by the Hungarian Partner between September 27 and 30 in Budapest. Over seventy members of the eight national nodes came together to review our common activity within the Network during the first year and to discuss further progress. In addition, we invited William H. Butler, Hiroshi Katayama-Yoshida and Antoine Georges who are leading researchers on the field relevant to the Network. In total fifty five oral contributions, among them six review talks, were sorted into several topical sessions.

Three sessions including fourteen contributions were devoted to *spin-dependent transport.* A comprehensive band-theoretical description of Fe|FeO|MgO|Fe tunneling junctions was given by William Butler illuminating also implications to the magnetoconductance properties. Experimental work of Martin Bowen *et al.* underlined the importance of the actual electronic structure of the insulating barrier to the spin-polarization of tunneling electrons. Ab initio calculations of the magnetoresistance of different Fe/Semiconductor/Fe junctions were presented by Voicu Popescu on the basis of the Drude model and in terms of the Kubo-Greenwood approach by Heike Herper. The Kubo linear response formalism to the interatomic transport was developed and applied to magnetic alloys by Ilja Turek *et al.,* while Mairbek Chshiev used an extension of the Kubo formalism to tunneling of asymmetric magnetic double barrier structures. Most contributions relied on a kind of the Landauer-Büttiker approach to tunneling. Josef Kudrnovský showed how to separate ballistic and diffusive parts of transport as well as effects of bulk and interface disorders. Peter Zahn presented first applications of a supercell approach to a periodic arrangement of electrodes and barriers of finite thicknesses. Olaf Wunnicke and Phivos Mavropoulos discussed different aspects of ballistic spin injection through Fe/SC/Fe junctions, predicting high polarization of the current due to symmetry of the corresponding electronic states and existence of quantum well states due to the reflection at both Fe/Sc interfaces. A novel promising transfer matrix approach based on a Green's function method within the FLAPW basis set was introduced by Daniel Wortmann. The influence of disorder

to tunneling magnetoresistance was studied by Maciej Zwierzycki *et al.* by using transmission matrices as calculated in terms of the TB-LMTO Green's function method for large lateral superlattices. Julie Grollier reported on experiments of magnetization reversal induced by spin-polarized current in Co/Cu/Co nano-pillars discussing among others the variation of the critical current with respect to the applied field. Finally, within a semiclassical approximation scheme, Gerrit Bauer gave a quick overview to the characteristics of magnetoelectronic circuits and devices, presenting also results for interface conductances as computed from first principles.

Half-metals are very promising potential candidates for applications in spinelectronics. Gillian Gehring highlighted the physics of manganites and discussed various problems, such as the ordering at different temperatures and compositions and the surface degradation, which can affect the tunneling magnetoresistance. By using XMCD experiments, the magnetic configurations in a new kind of half-metallic materials, namely, the double perovskites, were studied by Michael Besse *et al.* and compared to SIC-LSD calculations. These kind of calculations were then presented in more details by Dzidka Szotek, who predicted an anti-parallel alignment of the Fe and Mo moments both in Sr2FeMoO6 and Ba2FeMoO6, while Besse et al. experiments report anti-parallel alignment of these moments in Sr2FeMoO6 but parallel alignment in Ba2FeMoO6. Iosif Galanakis performed extensive first principles calculations on $C1_b$-type Heusler alloys and pointed out that a small modification of the lattice parameter or the presence of surface (interface) strongly influences the half-metallic character of these materials.

Ferromagnet/Superconductor interfaces represent an important and, concerning the underlying physics, challenging field of research of magnetoelectronic devices. Paul Kelly showed how a newly developed model based on the first principles TB-LMTO model can describe the Andreev reflection at FM/S interfaces allowing a detailed comparison with experiments. Daniel Huertas-Hernando demonstrated the feasibility the absolute spin-valve effect with superconducting proximity structures. As a preamble to the study of FM/S interfaces Mariusz Krawiec investigated 'normal metal/superconductor' double layers on the basis of a Hubbard model in the presence of a supercurrent flowing through the interface and discussed the characteristics of the ground state.

In terms of the KKR-CPA method, Hiroshi Katayama-Yoshida reported on systematic investigations of 3d-TM doped II-VI and III-V compound semiconductors. The purpose of these calculations was to design *ferromagnetic semiconductor* devices (e.g., spin-polarized FET, photo-induced magnetic memory) useful for technological applications. Lars Berquist showed that, for a range of concentrations of As defects in $(Ga_{1-x}Mn_x)As$, only a novel magnetic structure with partial disorder of the local moments is consistent with the magnetic moments measured experimentally. Supported by FLAPW calculations, František Máca proposed an explanation to the valence hole discrepancy problem in Mn-doped III-V semiconductors by making the assumption that some Mn atoms can occupy interstitial rather than substitutional positions in the crystal. The knowledge of the magnetic properties at the *ferromagnet/semiconductor interfaces* is of crucial impor-

tance to understand the actual TMR effect. For that reason, Fredrik Gustavsson performed XMCD and CEMS experiments on epitaxial Fe/ZnSe(001) heterostructures with Fe thickness ranging from submonolayer to bulk and found that the magnetic moment at the interface is preserved or even enhanced with respect to the Fe bulk value. Taking into account surface relaxations and reconstructions, Biplab Sanyal presented structural and magnetic studies of Fe/GaAs, Fe/Ge, Fe/ZnS and Fe/InAs interfaces, whereby for a proper understanding of the magnetic properties at the interface he also varied the thickness of Fe layers. Michal Kosuth *et al.* performed KKR-CPA calculations for $Fe_3(GaAs)_5$ and related superlattices observing appreciable induced magnetic moments in the semiconductor. In terms of first principles molecular dynamics calculations of the Fe/GaAs(100) interface, Voicu Crisan stressed that relaxation processes can strongly modify the charge transfer and the magnetization profile, while diffusion of As atoms into the Fe slab may also occur.

There is a considerable effort within the Network to study the properties of *magnetic films and multilayers* and, in particular, different *magnetic nanostructures*. Patrick Bruno presented recent calculations of the effective exchange interactions in Fe/Cu(100) and Co/Cu(100) monolayers covered by a Cu-cap of varying thickness, which have then been used as parameters of an effective Heisenberg-model. The variation of the Curie temperature calculated within the RPA was found in qualitative agreement with experiments. Similar oscillatory behavior of the Curie temperature with respect to the thickness of the Cu-cap was found by Julie Staunton *et al.*, who used a DLM approach to calculate the paramagnetic spin-susceptibility of the $Cu/Fe_n/Cu(100)$ system (n=2-8). Starting from the semi-phenomenological Landau-Lifshitz equation and a relativistic spin-polarized KKR theory, László Udvardi derived expressions for the spin-wave excitation energies including both exchange interactions and spin-orbit coupling and presented first results for thin magnetic films. By using the relativistic spin-polarized screened KKR method Silvia Gallego investigated the influence of the chemical environment of Mn atoms and the segregation of Pt from the bulk to the magnetic anisotropy of Mn/Pt multilayers, while Robert Hammerling systematically studied how the surface relaxation affects the MAE of ultrathin Co-films deposited on Cu(111). A spin-spiral model within the LMTO method has been applied by Bogdan Yavorsky to study the magnetoresistance due to Bloch walls in Fe as a function of the orientation of the magnetization, domain wall thickness and domain size. Based on calculations using different models in the framework of the KKR-ASA-CPA, Weine Olovsson concluded that the assumption of complete screening leads to quantitatively good comparison with experiments for the surface and interface core level shifts in the Mn/Pd(100) overlayer system. Nikos Papanikolaou presented ab initio calculations of the electronic structure and real-space conductance of freestanding nanowires. A Green's function embedding technique within the SKKR method has been used by Bence Lazarovits *et al.* to study small Fe, Co and Ni clusters on Ag(100) with special emphasis to magnetic anisotropy properties. Levente Vitos *et al.* investigated the energetics of Pd and Rh clusters and found that, consistent to recent experimental findings, small Pd clusters with non-crystallographic icosahedral symmetry exhibit ferromagnetic order.

(Regrettably, because of visa problems Valeri Stepanyuk and Dimitri Bazhanov could not participate the meeting and present their new results on 'Interaction energies of adatoms on metal surfaces' and 'Strain relief at metal interfaces', respectively.)

Antoine Georges gave us an exciting introduction to the Dynamical Mean Field Theory, which became an attractive tool to handle *correlated electron systems* over the past few years. General features of the approach were discussed with particular emphasis on how to merge it with first principles electronic structure calculations (LDA+DMFT) in order to deal with transition metal oxides, f-electron systems or even itinerant ferromagnets. As an example, Liviu Chioncel presented a generalization of the Exact Muffin-tin Orbitals approach in the framework of DMFT with test calculations on transition metals and their oxides. Vaclav Drchal introduced a multi-band Hubbard Hamiltonian on the basis of a TB-LMTO approach including disorder via CPA, whereas the correlation effects were described in terms of the fluctuating-exchange approximation, and showed applications to 3d metals and their disordered alloys. Arthur Ernst pointed out the need for taking into account screened Coulomb potential when studying the TMR effect and featured a scheme to calculate the polarization function within the RPA and the KKR Green's function method. Diemo Ködderitzsch applied the self-interaction corrected LSDA implemented within the TB-LMTO-ASA to NiO bulk and its (100) surface by investigating the stability of different antiferromagnetic orders and the trend of the exchange interaction constants from the bulk to the surface.

Different *spectroscopies*, in particular, the magneto-optical Kerr effect and the angle-resolved photoemission are important experimental tools to study magnetic materials. Alexander Perlov described the concept of layer-resolved optical conductivities exploited with a 'Baukasten principle' to calculate magneto-optical properties of complex layered systems, while he also introduced a more general scheme to a fully relativistic response theory in arbitrary order. By including multiple reflections and interferences on the boundaries in-between atomic layers, András Vernes has shown how to link the complex optical conductivity tensor calculated via the Kubo-Luttinger formalism within the SKKR method to the Kerr spectra of multilayer systems which can directly be compared with experiments and illustrated the theory for Co/Pt multilayers. Jan Minár presented fully relativistic KKR calculations of the resonant magneto-optical properties in the X-ray regime for disordered $Fe_{0.5}Ni_{0.5}$ and Co_xPt_{1-x} alloys and Fe/Ag and Pt/Co layered systems. Walter Temmermann featured an implementation of ARPES within the layer-KKR method treating the photo-current and self-consistency on the same footing and discussed, in particular, the effects of quantum well states to the photo-current in multilayers. By using ab initio molecular dynamics and the FLAPW method, Josef Redinger provided a detailed description of the electronic structure of realistic STM tips on a model of adsorbed 3d and 4d atoms on W(100).

Several contributions were dealing with different aspects of *magnetism of bulk and surface alloys*. Based on calculations with the TB-LMTO-CPA method, Peter Mohn put forward a new explanation to the weak ferromagnetism in $Y(Co_{1-x}Al_x)_2$ compounds ($0 \leq x \leq 0.25$)

and discussed the role of disorder and volume effects. In terms of the constrained local moment model and first principles spin-dynamics, Balázs Újfalussy investigated non-collinear magnetic states in large cells (up to 2048 atoms) of the γ-FeMn alloy, concluding that a randomly relaxed 3Q state can be more stable than the ideal one. Leonid Pourovskii *et al.* used a technique combining the screened generalized perturbation method with the Monte Carlo method to obtain the temperature of disorder-order transition in $Ni_{0.5}Pt_{0.5}$ as well as segregation profiles on the low-index surfaces of the NiPt and NiPd alloys. Hubert Ebert introduced the Augmented Space Method based on the KKR technique, which enables the treatment of impurities at interstitial sites in a crystal and presented hyperfine fields calculations of light interstitial impurities in Fe and Ni bulk. Diana Benea determined magnetic Compton profiles of different alloys from spin-polarized relativistic KKR bandstructure by pointing out that in particular cases it is indispensable to account for relativistic effects. Martin Friák calculated the tensile strength of iron for [100] loading by using the FLAPW method within the GGA and analyzed the structural and magnetic response to the loading. By performing total energy calculations along the displacive trigonal deformation path connecting bcc, sc and fcc structures, Dominik Legut investigated the influence of spin-orbit coupling to the elastic constants of Pb.

As rewied above, the research performed within the Network during the first year clearly covers a large variety of problems of magnetoelectronics and related topics. There is a vivid interaction between the members of the Network as also reported by the node leaders on the Management Meeting. This cooperation will be strengthened by numerous workshops and collaborative visits during the coming year. Most of the postdoc positions have already been occupied. The next annual meeting will be organized by the French node.

János Kollár & László Szunyogh

Programme

Sep 27, Thursday

13.55-14.00 **Opening** (*Peter Dederichs*)

Spin–dependent transport I.

14.00-14.45 **Calculated effects of the iron-oxide layer in Fe|FeO|MgO|Fe spin dependent tunneling junctions**
W. H. Butler, X.-G. Zhang, T.C. Schulthess, and J. M. MacLaren

14.45-15.00 **Large magnetoresistance in Fe/MgO/FeCo(001) epitaxial tunnel junctions on GaAs(001)**
M. Bowen, V. Cros, F. Petroff, A. Fert, C. Martínez Boubeta, J. L. Costa-Krämer, J. V. Anguita, A. Cebollada, F. Briones, J. M. de Teresa, L. Morellón, M. R. Ibarra, F. Güell, F. Peiró, A. Cornet

15.00-15.15 **Perpendicular transport in Fe/Semiconductor heterostructures**
H. C. Herper, L. Szunyogh, C. Blaas, P. Weinberger, and C. Sommers

Magnetism of alloys

15.15-15.30 **Formation of Weak Ferromagnetism in $Y(Co_{1-x}Al_x)_2$ Compounds: A CPA Study**
S. Khmelevskyi, I. Turek, and P. Mohn

15.30-15.45 **On the Magnetic Structure of γ–FeMn Alloys**
B. Újfalussy, G. M. Stocks, W. A. Shelton, T.C. Schulthess and A. Canning

15.45-16.00 **Bulk ordering and surface segregations in the NiPt and NiPd alloys**
L.V. Pourovskii, A.V. Ruban, I.A. Abrikosov, and B. Johansson

16.00-16.30 Coffee break

Half–metallic systems

16.30-17.15 **The Manganite Problems**
G. Gehring

17.15-17.30 **XMCD on bulk materials of A_2FeMoO_6 (A=Ba,Ca,Sr)**
M.Besse, A. Barthélémy, V. Cros, H. Jaffrès, J. Vogel, A. Mirone, D. Szotek, W. M. Temmerman, P. Berthet, P. Decorse, P. Bencock, A. Tagliaferri, N. Brookes, A. Rogalev, A. Revcolevschi, J.-P. Contour, A. Fert

17.30-17.45 **Electronic Structure of Correlated Transition Metal Oxides**
Z. Szotek, W.M. Temmerman, H. Winter and A. Svane

17.45-18.00 **Surface and Interface Magnetic Properties of Heusler Alloys**
I. Galanakis, N. Papanikolaou, and P.H. Dederichs

19:00 Dinner

Ferromagnet/superconductor interfaces

9.00- 9.45 **The transmission polarization of ferromagnet/superconductor interfaces**
K. Xia, P.J. Kelly, G.E.W. Bauer, and I. Turek

9.45-10.00 **Absolute spin-valve effect with superconducting proximity structures**
D. Huertas-Hernando, Yu.V. Nazarov, and W. Belzig

10.00-10.15 **Diamagnetic Response of Normal metal – Superconductor Interfaces**
M. Krawiec, J.F. Annett, and B.L. Györffy

10.15-10.45 Coffee break

Spin–dependent transport II.

10.45-11.00 **Ab initio calculations of magnetoresistance, interlayer exchange constants and magneto-optical properties of the ferromagnet-semiconductor layered systems Fe/GaAs and Fe/Ge**
V. Popescu, A. Perlov, and H. Ebert

11.00-11.15 **Ab initio theory of perpendicular transport in layered magnetic systems**
J. Kudrnovský, V. Drchal, I. Turek, P. Dederichs, P. Weinberger, and P. Bruno

11.15-11.30 **Supercell approach and tunnel conductance**
Peter Zahn, Ingmar Riedel, and Ingrid Mertig

11.30-11.45 **Ballistic Spin Injection from Fe into ZnSe and GaAs**
O. Wunnicke, Ph. Mavropoulos, R. Zeller, and P.H. Dederichs

11.45-12.00 **Ballistic Spin Injection through Fe/SC/Fe Junctions**
Ph. Mavropoulos, O. Wunnicke, N. Papanikolaou, R. Zeller, and P.H. Dederichs

12.00-12.15 **A transfer matrix method for ballistic transport: MgO/Fe(001)**
D. Wortmann, G. Bihlmayer, S. Blügel, and H. Ishida

12.30 Lunch

Spin–dependent transport III.

14.00-14.15 **Magnetoresistance effects in disordered bulk alloys by means of the TB-LMTO-CPA method**
I. Turek, J. Kudrnovský, V. Drchal, L. Szunyogh, P. Weinberger, and P.H. Dederichs

14.15-14.30 *Ab initio* **calculations of tunneling magnetoresistance**
M. Zwierzycki, K. Xia, P.J. Kelly, G.E.W. Bauer, and I. Turek

14.30-14.45 **Spin-Polarized Transport in Magnetic Double Barrier Junctions**
M. Chshiev, D. Stoeffler, C. Tiusan, A. Vedyayev and K. Ounadjela

14.45-15.00 **Magnetization reversal induced by spin polarized current**
J. Grollier, V. Cros, H. Jaffrès, J.M. George, A. Hamzic, G. Faini, J. Ben Youssef, H. Legall, A. Fert

15.00-15.15 **Theory of spin transport across hetero-interfaces**
G.E.W. Bauer, Yu.V. Nazarov, D. Huertas-Hernando, K. Xia, P.J. Kelly, and A. Brataas

Spectroscopy

15.15-15.30 **Theoretical description of the magneto-optical properties of arbitrary layered systems**
A. Perlov, T. Huhne, and H. Ebert

15.30-15.45 **Kerr spectra calculated for multilayer systems**
A. Vernes, L. Szunyogh, and P. Weinberger

15.45-16.00 **Theoretical description of resonant magneto-optical properties in the X-ray regime**
J. Minár and H. Ebert

16.00-16.30 Coffee break

16.30-16.45 **Ab initio calculations of angle-resolved photoemission spectra in multiple scattering**
M. Lüders, A. Ernst, W. M. Temmerman, Z. Szotek

16.45-17.00 **Modeling STM tips by single absorbed atoms on W(100) films: 3d and 4d transition metal atoms**
W. A. Hofer, J. Redinger, and R. Podloucky

17.00-18.30 **Management Meeting; Round-table discussion**

19.00 Dinner

Sep 29, Saturday

Ferromagnetic semiconductors, Ferromagnet/semiconductor interfaces

9.00-9.45 **Ab-initio calculation and materials design of ferromagnetic semiconductors**
H. Katayama-Yoshida and K. Sato

9.45-10.00 **Defect induced partial magnetic order in $(Ga_{1-x}Mn_x)As$**
L. Bergqvist, P. A. Korzhavyi, E. A. Smirnova, I. A. Abrikosov, P. Mohn, R. Mathieu, P. Svedlindh, J. Sadowski, and O. Eriksson

10.00-10.15 **Mn impurities in GaAs and GaP crystals**
F. Máca and J. Mašek

10.15-10.30 **Interface magnetic properties of epitaxial Fe/ZnSe(001) heterostructures**
F. Gustavsson, J.M. George, V. Cros, F. Petroff, A. Fert, E. Nordström, V. H. Etgens, M. Marangolo, and M. Eddrief

10.30-11.00 Coffee break

11.00-11.15 **First principles study of ferromagnet-semiconductor interfaces**
B. Sanyal and S. Mirbt

11.15-11.30 **Electronic and magnetic properties of Fe on GaAs(100) surfaces**
M. Košuth, H. Ebert, and H. Akai

11.30-11.45 **A first-principles molecular dynamics study of the Fe/GaAs(001) interface**
V. Crisan, P. Entel, and H. Ebert

11.45-12.00 *Ab initio* **study of the electronic and magnetic structure of the NiO(100) surface**
D. Ködderitzsch, W. Hergert, Z. Szotek, and W.M. Temmerman

12.00-12.15 **Calculation of hyperfine fields of light impurities at interstitial lattice sites in ferromagnetic metals**
Ch. Zecha, H. Ebert, P. H. Dederichs, and R. Zeller

12.30 Lunch

Magnetic films and multilayers

14.00-14.45 **Oscillatory Curie Temperature of Two-Dimensional Ferromagnets**
M. Pajda, J. Kudrnovský, I. Turek, V. Drchal, and P. Bruno

14.45-15.00 **The onset of magnetic order in fcc-Fe films on Cu(100)**
J.B. Staunton, S.S.A. Razee, L. Szunyogh and B.L. Györffy

15.00-15.15 **Theoretical study on non–collinear magnetic structures by means of fully relativistic KKR method**
L. Udvardi, L. Szunyogh, K. Palotás, and P. Weinberger

15.15-15.30 **Magnetic anisotropy of ordered and disordered Mn/Pt multilayers**
S. Gallego, M.C.Muñoz, J.Zabloudil, L.Szunyogh, P.Weinberger

15.30-15.45 **Magnetic anisotropy of ultrathin Co-films on Cu(111) including relaxation effects**
R. Hammerling, L. Szunyogh, J. Zabloudil, C. Uiberacker, and P. Weinberger

15.45-16.00 **Giant Magnetoresistance due to a domain wall in Fe:** *Ab initio* **study**
B.Yu. Yavorsky and I.Mertig

16.00-16.30 Coffee break

Magnetic nanostructures

16.30-16.45 **Surface Core Level Shift in PdMn systems on Pd(100) by the model of Complete Screening**
W. Olovsson, I. Abrikosov, and B. Johansson

16.45-17.00 **Ab initio calculated electronic structure of metallic nanowires**
N. Papanikolaou, J. Opitz, P. Zahn, and I. Mertig

17.00-17.15 **Magnetic properties of adatoms and small clusters on metallic surfaces**
B. Lazarovits, L. Szunyogh and P. Weinberger

17.15-17.30 **Magnetic properties and stability of palladium and rhodium nanoclusters**
L. Vitos, J. Kollár and B. Johansson

19.00 Banquet

Sep 30, Sunday

Correlated systems

9.00- 9.45 **Introduction to the Dynamical Mean Field Theory of correlated systems and its implementation in electronic structure calculations**
A. Georges

9.45-10.00 *Ab – initio* **electronic structure calculations of correlated systems**
L. Chioncel, L. Vitos, I.A. Abrikosov, and A.I. Lichtenstein

10.00-10.15 **Electron correlations in metallic systems**
Václav Drchal, Josef Kudrnovský, and Václav Janiš

10.15-10.30 **Properties of the screened Coulomb potential in TMR materials**
A. Ernst, M. Lüders, P. Bruno, W.M. Temmerman, and Z. Szotek

10.30-11.00 Coffee break

Bulk phenomena

11.00-11.15 **A relativistic description for the magnetic Compton scattering of solids**
D. Benea and H. Ebert

11.15-11.30 **Calculation of tensile strength in iron from first principles**
M. Friák, M. Šob, and V. Vitek

11.30-11.45 **Spin-orbit coupling and higher-energy phases in Pb along the trigonal deformation path**
D. Legut, M. Friák, and M.Šob

11.45-11.50 **Closing remarks** (*Walter Temmerman*)

12.30 Lunch

Abstracts

Partner United Kingdom

The Manganite Problems

Gillian A. Gehring

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The oxide magnets do have a number of very different propertis from the well known transition metals. The physics behind this are explained briefly. The current problems relate to the variety of ordering seen at different temperatures and compositions and surface degredation which affects the TMR. The experimental background and the ways in which computational physics can contribute to the physical understanding are reviewed.

Electronic Structure of Correlated Transition Metal Oxides

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The self-interaction corrected local spin density approximation is applied to magnetite (Fe_3O_4) and such double perovskites as Sr_2FeMoO_6 and Ba_2FeMoO_6. Issues of charge ordering in magnetite, and electronic and magnetic structures are discussed. In agreement with experiment, a large magnetic moment of $\sim 0.4\ \mu_B$ is calculated for Mo. In both perovskites the Fe and Mo calculated magnetic moments are anti-parallel with respect to one another, in contradiction to experiments, finding them to be parallel in the Ba-compound.

Ab initio calculations of angle-resolved photoemission spectra in multiple scattering

M. Lüders[a,b)], A. Ernst[c)], W. M. Temmerman[a)], Z. Szotek[a)]

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[c)] *Max-Planck Institut für Mikrostrukturforschung, Halle, Germany*

We present an implementation of photoemission within the layer-KKR method, allowing a treatment of the photo-current and the self-consistent potentials on the same footing.

It will be demonstrated how the the obtained photoemission spectra can be analyzed by comparing with layer resolved spectral functions. This method will be applied to calculate the photocurrents of magnetic multilayers where especially the features due to the quantum well states will be discussed.

The onset of magnetic order in fcc-Fe films on Cu(100)

J.B. Staunton[a)], S.S.A. Razee[a)], L. Szunyogh[b)] and B.L. Györffy[c)]

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On the basis of a first-principles electronic structure theory of finite temperature metallic magnetism in layered materials, we investigate the onset of magnetic order in thin (2-8 layers) fcc-Fe films on Cu(100) substrates. The nature of this ordering is altered when the systems are capped with copper. Indeed we find an oscillatory dependence of the Curie temperatures as a function of Cu-cap thickness, in excellent agreement with experimental data. The thermally induced spin-fluctuations are treated within a mean-field disordered local moment (DLM) picture and give rise to layer-dependent 'local exchange splittings' in the electronic structure even in the paramagnetic phase. These features determine the magnetic intra- and interlayer interactions which are strongly influenced by the presence and extent of the Cu cap.

Diamagnetic Response of Normal metal-Superconductor Interfaces

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We study the ground states of a 'normal metal – superconductor' double layer on the basis of a simple Hubbard Model whose 'on site' interaction parameter, U, is positive (U_+) on one (normal metal) side and negative (U_-) on the other (superconducting) side of the interface separating the two layers. We allow for a spontaneously generated supercurrent to flow in the interface and solve the Hartree-Fock-Bogoliubov-deGennes equation coupled to the full Maxwells equation (in particular Amperes Law) fully selfconsistantly. The calculation is carried out using the 'principle-layer' method for systems of 50 to 100 layers of infinite 2d square lattices and we find that, for both U_+ and U_- non-zero, the ground state features a finite supercurrent in agreement with the results of semi-classical theory [1,2] and experiments[3]. We shall discuss the salient characteristics of this remarkable

state and speculate on the outcome of the next step of our project which is the study the case where the normal metal is ferromagnetic.

[1] G. Deutscher and P.G. de Gennes,in SUPERCONDUCTIVITY (ed. by R.D. Parks), (Marcel Dekker, New York, 1969)
[2] C. Mota, P. Visani, A. Pollini, and K. Aupke, Physica B **197**, 95 (1994)
[3] W. Belzig, C. Bruder, and Gerd Schon, Phys. Rev. B **53**, 5727 (1996)

Partner Germany-I

Surface and Interface Magnetic Properties of Heusler Alloys

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We have studied the magnetic properties of the $C1_b$-type [XMnSb (X=Co,Ni,Pd,Pt)] and of the $L2_1$-type [Co_2MnZ (Z=Al,Si,Ga,Ge,Sn,Sb)] Heusler alloys. The calculations apply density functional theory in the local density approximation and the screened KKR Green's function method. All these compounds are strong ferromagnets with high Curie temperatures that makes them promising for magnetoelectronic applications. NiMnSb, PtMnSb, Co_2MnSi and Co_2MnGe are half-ferromagnets, i.e. they possess a semi-conducting spin-down band, and thus they present 100% spin-polarization at the Fermi level. All the other studied compounds also have a gap in the spin-down band but the Fermi level is slightly below or above the gap. We show that a small contraction or expansion of the lattice parameters provokes a rigid shift of the bands and thus the Fermi level moves inside the gap. We study the low-index surfaces of these compounds taking into account different terminations. The surfaces exhibit strong deviations from the bulk electronic structure and the half-ferromagnetic character can be lost.

Ballistic Spin Injection through Fe/SC/Fe Junctions

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[b)] *Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, Fachgruppe Theoretische Physik, D-06099 Halle, Germany*

We report a theoretical study of spin injection through perfect epitaxial Fe/SC/Fe junctions, where SC stands for the semiconducting materials ZnSe, GaAs, and InAs. Our approach is based on a Local-Density-Functional KKR Green's function method. The conductance is calculated in the linear-response limit using a Landauer-like formula for the ballistic regime. Two independent spin channels are assumed; spin-flip or diffuse

scattering are not taken into account. A "gate" voltage is modeled through artificial lowering of the SC potentials, so that the Fermi level will lie slightly in the conduction band. Our results show a definite dependence of the current polarization on the SC thickness, approaching 100% for large thicknesses. Three interesting aspects appear. Firstly, the symmetry matching between the Fe and SC states, enhancing the importance of the current near and at the $\bar{\Gamma}$-point of the surface Brillouin zone. Secondly, the possible modification of the SC energy bands under epitaxial tetragonalization, which might bring bands far away from the $\bar{\Gamma}$-point into play as well. And thirdly, the existence of quantum well states due to the reflection at both Fe/SC interfaces.

A transfer matrix method for ballistic transport: MgO/Fe(001)

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The tunnel-magneto resistance (TMR) effect has been extensively studied in the last couple of years. The complicated interplay between electronic structure, atomic structure and the tunneling process through the tunnel barrier makes a theoretical description beyond idealized models very challenging. The FLAPW-method is an excellent tool to determine the relaxation and the electronic structure of oxides and semiconductors in contact with magnetic materials. However, the description of transport properties seems less natural within the FLAPW method as in the KKR method for example, which is based on a scattering formalism.

We present a new transfer matrix method which overcomes this limitation. From the transfer matrix, both the complex band structure and the transmission coefficients, needed in the Landauer-Büttiker formulation of ballistic transport, are easily obtained. The method is based on a Green's function formalism within the FLAPW basis set. Both the theory and a first application to the structurally relaxed Fe(001)/MgO/Fe(001) tunnel-junction will be discussed.

Ballistic Spin Injection from Fe into ZnSe and GaAs

O. Wunnicke, Ph. Mavropoulos, R. Zeller, and P.H. Dederichs

Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

We have investigated by *ab initio* calculation the ballistic spin injection from a Fe (001) halfcrystal into ZnSe and GaAs crystals. The results show that in the ballistic limit a very high spin polarization ($> 90\%$) can be achieved.

The calculations are performed by the *ab initio* KKR method and the Landauer formalism for the conductance using a Green's function expression of Baranger and Stone. We

describe the injection by three models: (i) the injection of hot Fe states, (ii) the injection into the conduction band being lowered by a sharp potential step, and (iii) injection through a smooth potential barrier.

We study the polarization of the injected spin current for different energies above the conduction band minimum and for different interface terminations. In the cases (i) and (ii) we always obtain very high polarization, sometimes as high as 98%. The high polarizations can be explained by the symmetry of the Fe states in the majority and minority bands and their coupling to the conduction band states of the semiconductor. Somewhat lower polarizations can occur in the barrier model, when the tunneling through the barrier is dominated by the Fe interface states in the minority band.

We discuss the importance of these results for the spin transistor proposed by Datta and Das [Appl. Phys. Lett. **56**, 665 (1990)].

Calculation of hyperfine fields of light impurities at interstitial lattice sites in ferromagnetic metals

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Even though substitutional impurities have been investigated quite intensively from a theoretical point of view, there are comparatively few corresponding investigations concerning impurities on interstitial lattice sites. An important example consists in light interstitials implanted in ferromagnetic metals. Here the magnetization of the host atoms induces a hyperfine field at the impurity atoms, which themselves are normally unmagnetic. However, calculations of the hyperfine fields in Fe and Ni frequently yield strong deviations from the experimental results, which have commonly been ascribed to the relaxation of the nearest neighbouring atoms. Nevertheless, the influence of the lattice distortion has been disregarded so far. A method which has been presented recently and which is based on the KKR bandstructure method allows to embed the impurity in the crystal and to account for the lattice distortion with high accuracy. The calculated hyperfine fields of the impurities of the first and second period in Fe and Ni are presented and the influence of structural disorder is discussed.

Ab initio calculations of magnetoresistance, interlayer exchange constants and magneto-optical properties of the ferromagnet-semiconductor layered systems Fe/GaAs and Fe/Ge

Voicu Popescu, Alexander Perlov and Hubert Ebert

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The deposition of magnetic materials on semiconductors allowed the synthesis of a number of new artificial materials with potential applications in magneto-electronics. In particular ferromagnetic-semiconductor (FM/SC) heterostructures have a potential use in devices based on the TMR (tunneling magneto-resistance). We report results of calculations of the electronic, magnetic, transport and magneto-optical properties of Fe/GaAs and Fe/Ge multilayer systems that are meant to model FM/SC/FM trilayer systems.

On the base of the generalized Bloch theorem [1] we have calculated the electronic structure of a set of spin-spiral structures, which allows us to extract averaged interlayer exchange parameters and their dependence on the width of the semiconductor spacer. Also the dependence of the dc conductivity and magneto-resistance on the width of the semiconductor layer and the relative angle between magnetic moments is presented and discussed. These are calculated on the basis of the Drude model for ballistic and diffusive regimes.

Spatially resolved optical conductivity spectra (both diagonal and off-diagonal parts) which provide information about spatial profiles of optical constants are presented as well. These spectra allow to investigate in detail the spatial origin of magneto-optical properties of layered systems. In addition, on the base of these data taking advantage of the so-called Baukasten principle [2] the complex Kerr rotation spectra both for multilayer and trilayer FM/SC/FM systems are calculated.

All calculations have been done in the framework of local density approximation to the density functional theory.

[1] C.Herring, in "Magnetism", vol. 4, ed. by G. T. Rado and H. Suhl, Academic Press, New York (1966)
[2] A. Perlov and H. Ebert, Europhys. Lett. **52**, 108 (2000)

Theoretical description of the magneto-optical properties of arbitrary layered systems

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The calculation of the optical properties of ordered solids can nowadays be done in a more or less routine way. Even the magneto-optical effects caused by the interplay of magnetism and spin-orbit coupling can be investigated in a quantitative way by using modern methods of band structure calculation. However, the interpretation of the corresponding magneto-optical spectra is by no means straightforward. In addition, there are still several important classes of materials that are not accessible to ab initio type investigations.

To allow for a detailed analysis of the magneto-optical properties of periodic magnetic multilayer systems, the concept of the layer-resolved optical conductivity applied by means of a conventional band structure method is introduced. It will be shown that the layer

projected optical conductivity of an atomic layer is influenced by only very few neighboring layers. This property can be exploited with the Baukasten principle that aims to predict the magneto-optical properties of a complex layer system from the properties calculated for a closely related but simpler one.

In addition, a more general scheme will be introduced that allows to define the frequency-dependent optical conductivity tensor for arbitrary layered systems in a layer-resolved way. This opens in particular the way to deal with the magneto-optical properties of magnetic surface layer systems and to calculate the corresponding magneto-optical Kerr spectra. The formalism, based on a fully relativistic description of response theory in arbitrary order, will be described in short results for surface layer systems will be presented.

Electronic and magnetic properties of Fe on GaAs(100) surfaces

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The electronic and magnetic properties of ferromagnet-semiconductor heterostructure multilayer systems have been studied by means of scalar-relativistic KKR-CPA band structure calculations. Concerning the resulting magnetisation profiles of $Fe_3/(GaAs)_5$ and other related systems the most important features are that no magnetically dead layers occurred and an appreciable induced magnetisation was found in the semiconductor subsystem. By investigation of the hyperfine interaction more detailed information on the electronic structure could be obtained. Properties of related compounds (Fe_2As, Fe_3GaAs,...), possibly occuring at the Fe/GaAs interface, were investigated.

The work has been based so far on unrelaxed ferromagnet-semiconductor heterostructures. In the near future investigations of the influence of lattice relaxations and imperfections will be main issue of the project. First results for a relaxation of the interlayer distance at the interface have been obtained. For As- as well as Ga-terminated semiconductor layers an expansion by around 4% has been found. This is accompanied by an increase of the Fe-moments at the interface.

Theoretical description of resonant magneto-optical properties in the X-ray regime

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A version of the Kubo-formula is presented, that allows to calculate the resonant magneto-

optical properties in the X-ray regime for arbitrary materials. This is achieved by representing the underlying electronic structure in terms of the Green's function. Calculating the Green's function in the framework of spin-polarised relativistic multiple scattering theory (SPR-KKR) in particular gives access to spin-orbit induced resonant magneto-optical properties. As for the optical regime of light, all magneto-optical properties in the X-ray regime are closely related to the optical conductivity. Our method for calculating of the frequency dependent optical conductivity allows therefore a rather detailed discussion of all experimentally observable magneto-optical phenomena.

Using the Green's function formalism allows in a straightforward way to deal with systems without three-dimensional translational symmetry. Two important examples for these are surfaces and disordered alloys. For the later case we present results of calculations of the Faraday effect for the $L_{2,3}$-edge of Fe and Ni in the disordered alloy $Fe_{0.5}Ni_{0.5}$ making use of the CPA. For the disordered alloy system Co_xPt_{1-x} the same effect has been studied at the L_3-edge of Pt for the whole concentration range. Using these results, in particular the relationship of the complex refractive index with the magnetic of the probed atom, will be discussed in some details. Also the results of calculations for the X-ray resonant scattering – transverse Kerr effect – in the layered systems Fe/Ag and Pt/Co will be presented.

A relativistic description for the magnetic Compton scattering of solids

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A fully relativistic formulation for the of spin resolved momentum density is presented together with a corresponding scheme to determine the magnetic Compton profiles for magnetic solids. This formalism is set up within the framework of spin-polarised relativistic Korringa-Kohn-Rostoker (SPR-KKR) method of bandstructure calculations. The development can be seen as a first step towards a fully relativistic treatment of magnetic Compton scattering. The results for computed directional magnetic profiles of Fe and Ni, where the relativistic effects are small, are presented and compared with nonrelativistic calculation of other larges and experimental data. The effects of disorder on the momentum density are studied making use of the Coherent Potential Approximation (CPA) and the corresponding computed Compton profiles for ordered and disordered Fe–Pt alloys are presented. The influence of the spin-orbit coupling is evidenced by scalar-relativistic/fully relativistic calculations of Compton profile in Gd and Y-Gd alloys. The calculated spectra shows good agreement also for a more demanding system, like UFe_2 where it is indispensable to account for relativistic effects.

Partner Germany-II

Oscillatory Curie Temperature of Two-Dimensional Ferromagnets

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The effective exchange interactions of magnetic overlayers Fe/Cu(001) and Co/Cu(001) covered by a Cu-cap layer of varying thickness were calculated in real space from first principles. The effective two-dimensional Heisenberg Hamiltonian was constructed and used to estimate magnon dispersion laws, spin-wave stiffness constants, and overlayer Curie temperatures within the mean-field and random-phase approximations. Overlayer Curie temperature oscillates as a function of the cap-layer thickness in a qualitative agreement with a recent experiment.

Properties of the screened Coulomb potential in TMR materials

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The study of the tunnel magneto-resistance (TMR) effect on the base of many-body physics involves using of the screened Coulomb potential, which plays a central role in a variety of phenomena. Here we present calculations of the screened Coulomb potential in some materials used in the TMR. The polarization function needed to evaluate the screened Coulomb potential is calculated within the random phase approximation (RPA), which corresponds to neglecting the vertex correction and using a non-interacting Green's function. We used the Korringa-Kohn-Rostoker (KKR) within the local density approximation (LDA) to evaluate the non-interacting Green's function. The screened Coulomb potential is represented in a local basis and can be easily implemented into further model calculations.

Supercell approach and tunnel conductance

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[b] *Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany*

We use a Screened-KKR-Green's-function method to calculate the electronic structure of tunnel junctions selfconsistently. By means of a supercell approach a periodic arrangement

of electrodes with finite thickness separated by identical barriers is considered. For the conductance the Landauer formula is evaluated in the ballistic limit for zero bias.

The consequences of the periodic boundary conditions on the transport properties will be discussed using an analytical free electron model. To get over the periodic boundary conditions in the transport calculation an inverse Kronig-Penney-model [1] was developed. The scattering properties of one barrier are derived from the eigenstates of the periodic supercell. First applications of this formalism to tunnel junctions will be presented.

[1] Ingmar Riedel, Peter Zahn, and Ingrid Mertig, Phys. Rev. B **63**, 195403 (2001)

Ab initio calculated electronic structure of metallic nanowires

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We will present ab initio calculations of the electronic structure of freestanding nanowires. The calculations are based on density functional theory using a Screened Korringa-Kohn-Rostoker method. The nanowires have a cross section of 4 up to 100 atoms. We assume a translational invariance in the direction of the wires. The thickness dependence of the band structure and the density of states (DOS) will be discussed. The electronic structure clearly shows features of the one dimensional system, that is, mini-bands due to quantum confinement and $1/\sqrt{E}$-singularities in the DOS. We will present preliminary results for a real-space conductance calculation along the wire direction.

Ab initio study of the electronic and magnetic structure of the NiO(100) surface

D. Ködderitzsch[a)], W. Hergert[a)], Z. Szotek[b)], and W.M. Temmerman[b)]

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[b)] *Daresbury Laboratory, UK*

An adequate description of strongly correlated systems, such as the antiferromagnetic insulating transition-metal monoxides (FeO, CoO, NiO), is not possible within the local spin density approximation to the density functional theory (LSDA-DFT) due to its mean-field treatment of the strong on-site Coulomb correlations. A better representation of the latter can be obtained within the self-interaction corrected (SIC) LSDA.

In this work we apply the self-interaction corrected LSDA formalism, as implemented in the TB-LMTO-ASA method, to study the electronic and magnetic structure of NiO(100).

We have modelled the surface in a supercell approach by a series of repeated slabs consisting of up to seven layers of oxide separated by five layers of empty spheres representing the vacuum. We discuss the layer resolved density of states and consider different arrangements of spin orientations in the surface layers whilst keeping the inner layers in AFII ordering.

Having investigated different magnetic orderings in the bulk and in the slabs we argue that the AFII phase is most energetically favoured.

In a further step we determine by fitting to a Heisenberg-model the nearest neighbour and next nearest neighbour exchange interaction constants in this system and extract trends in the change of the exchange constants when going from the bulk to the surface.

Giant Magnetoresistance due to a domain wall in Fe: *Ab initio* study

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The magnetoresistance due to a domain wall (DW) in pure Fe was studied theoretically by means of *ab initio* electronic structure calculations based on a linear muffin-tin orbital (LMTO) method modified for non-collinear magnets. The Bloch walls were modeled by a superlattice structure in (001) direction of the BCC lattice with alternating regions of collinear and spiral-like magnetisations. The conductivity was calculated by means of the linearized Boltzmann equation in a relaxation time approximation. The "current in the plane" (CIP) and the "current perpendicular to the plane" (CPP) magnetoresistance due to a DW is presented as a function of the angle between the magnetisations, domain wall thickness, and domain size. The orientation dependence of the magnetoresistance due to a DW in pure Fe has *cos*-like behavior in contrary to the giant magnetoresistance (GMR) in Fe/Cr superlattices. It was also shown that the presence of Cr increases the amplitude of the effect. The Kronig-Penney model was used in order to show that the oscillations of GMR as a function of domain size stem from quantum well states crossing the Fermi level.

Partner France

XMCD on bulk materials of A_2FeMoO_6 (A=Ba,Ca,Sr)

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Half-metallic materials are currently a hot topic in magnetism due to their high polarisation and to the possible applications with magnetoresistive tunnel junctions. The double perovskite family $A_2B'B''O_6$ (A = Ba, Sr, Ca and B'B" = FeMo, FeRe, CrMo) is very promising for applications as some compounds have a Curie Temperature that far exceeds the room temperature (Tc $\sim$ 410-450K with Sr_2FeMoO_6). Band structure calculations have shown that SFMO is half-metallic [1] and a large intergrain magnetoresistance have been found at room temperature in polycrystals [2]. Nevertheless, conduction mechanisms and magnetism in these systems remain unclear. A simple model suggests an antiferromagnetic order between Fe^{3+} and Mo^{5+} with a super-exchange interaction, which gives a four μ_B moment per formula unit. For Kobayashi et al., more detailed calculations give a moment of 3.8 μ_B on Fe and -0.3 μ_B on Mo.

We have performed X-ray Magnetic Circular Dichroism experiments (XMCD) at the $L_{2,3}$ edges of Fe and Mo on powders of BFMO, CFMO and SFMO, and monocrystals of SFMO. Thanks to its chemical selectivity, XMCD is able to measure the intensity of the individual magnetic moments on Fe and Mo, and also their relative orientation.

We have studied both powder and monocrystal of SFMO. Using sum rules, we have evaluated a spin moment of 3.2 μ_B on Fe site and -0.4 μ_B on Mo site for bulk powder (respectively 3.6 μ_B and -0.35 μ_B for monocrystal). Moreover, areas of dichroic signal of Fe and Mo have an opposite sign, which corroborates the idea of an antiferromagnetic order due to super-exchange. With atomic multiplet calculations, we found a proportion of 60 % Fe^{2+} ions for 40 % Fe^{3+} ions. These respective contributions are coherent with the results found by Mössbauer spectroscopy [3]. Moreover, among Fe^{2+} ions, a part has a low spin component, which is incompatible with the half-metallic character of the material. XMCD measures on CFMO and BFMO powders show varying absorption curves with the cation. These results can be explained by some modifications of the electronic structure due to the different size of the cations which induces a lattice distortion. But more surprisingly, contrary to SFMO, we found the same sign for the dichroic signal in CFMO and BFMO, hence a ferromagnetic coupling between Fe and Mo in these compounds. To better understand the difference of the magnetic configuration in these two materials, SIC-LSD calculations (self-interaction correction to local spin density) have been recently performed. The absolute values of the spin and orbital magnetic moments are in good agreement with experiments: 3.8 μ_B for Fe and -0.4 μ_B for Mo (BFMO compound) 3.69 μ_B for Fe and 0.42 μ_B for Mo (SFMO compound) but one finds an antiparallel arrangement between Fe and Mo for both compounds. Then, we still have a discrepancy between the theoretical calculations and experimental results.

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Large magnetoresistance in Fe/MgO/FeCo(001) epitaxial tunnel junctions on GaAs(001)

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The magnetoresistance of magnetic tunnel junctions (MTJs) is of uncontested interest for important applications with, in particular, promising perspectives for the fabrication of nonvolatile memories (MagneticRAM). Up to now, most studies have been performed on MTJs in which the insulating barrier between the ferromagnetic electrodes is a layer of amorphous alumina. MTJs with alumina provide large and reproducible tunneling magnetoresistance (TMR). However, to understand the physical mechanisms of spin-dependent tunneling, a transport study through an amorphous insulator is hardly accessible in a theoretical approach. Towards this end, much work has been expended to characterize the growth and electrical behavior of ultrathin MgO layers [1].

Here, we present experimental results showing large TMR values in Fe(001)/MgO(001)/-FeCo(001) epitaxial tunnel junctions grown by a combination of laser ablation and triode sputtering onto MgO-buffered GaAs(100). As evidenced by RHEED, x-ray diffraction and TEM analyses, optimized growth conditions result in entirely epitaxial samples of high crystalline quality with flat, sharp interfaces [2]. Fe(100)/MgO(20)/FeCo(100) junctions show up to 60% TMR at 30K, to be compared with 13% obtained recently by Yuasa et al. on (100)-oriented Fe/amorphous-Al2O3/FeCo tunnel junctions [3]. This difference demonstrates that the spin polarization of tunneling electrons can not be directly correlated with the spin-polarized DOS of a free metal surface, but depends on the actual electronic structure of the barrier/electrode system. Furthermore, we construe from the bias dependence of the TMR, previous experimental results and recent calculations [4] that s-character electrons are predominantly tunneling in the case of a 20Å MgO(100) barrier.

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Interface magnetic properties of epitaxial Fe/ZnSe(001) heterostructures

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A conventional magnetic tunneljunction (MTJ) consists of two ferromagnetic materials separated by a thin non-magnetic barrier. Depending on the relative orientation of magnetisation between the ferromagnetic electrodes, a change in resistance is observed and referred to as tunnel magnetoresistance (TMR).

A parameter of crucial importance for the magnitude of TMR is the spin polarisation defined as the spin asymmetry in the density of states at the Fermi level of the ferromagnets. Due to charge redistribution between the ferromagnet and the barrier during bond formation, the interface polarisation can differ significantly from that of bulk. Moreover, it is the interface polarisation that is transmitted in the tunneling process and determines the TMR. The use of a semiconductor tunnel barrier in heteroepitaxy with ferromagnetic metal electrodes would describe a novel type of MTJ's that integrate spin electronics with semiconductors. Many metal/semiconductor interfaces such as Fe/GaAs, however, are unstable to chemical reactions resulting in a risk of obtaining magnetically dead layers in proximity of the interface. The persistence of the bulk magnetic moment at the interface is therefore of importance for the TMR since a vanishing magnetic moment would give no spin polarisation.

Here we present a detailed study of the magnetic properties of Fe grown epitaxially on ZnSe(001) by MBE with Fe thickness ranging from submonolayer to bulk. ZnSe is a wide gap (2.8 eV) semiconductor with a zincblende structure and matches within 1% twice the lattice parameter of Fe. The magnetic moment near the interface has been probed by two alternative methods suitable for this purpose; X-ray magnetic circular dichroism (XMCD) and conversion electron Mössbauer spectroscopy (CEMS). Both methods show that the magnetic moment is preserved or even enhanced in the very first monolayers compared to the bulk value of Fe, which is inline with an interface stable against chemical reactions.

Magnetization reversal induced by spin polarized current

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A spin-polarized current can reverse the magnetic moment of a ferromagnetic layer, without the help of any magnetic field. This effect was first predicted in 1996 by Slonczewski [1]. His approach is ballistic, dynamic, and based on spin transfer between a thick (spin polarizer) and a thin ferromagnetic layer. Other models have been developed since, involving similar approaches [2] or different mechanisms [3]. Magnetization reversal induced by spin polarized current has been confirmed by recent experiments on nano-pillars at Cornell's University [4] and at Orsay [5].

We will present our latest experiments obtained on Co/Cu/Co nano-pillars. These structures present Current Perpendicular to Plane Giant Magnetoresistance (CPP-GMR) which allows us to differentiate between parallel (P) and antiparallel (AP) magnetic configurations of the Co layers. We find that a positive current switches the magnetization of the thin layer to a P configuration whereas a negative one switches it to AP configuration. This asymmetry is the signature of reversal by spin injection, as opposed to what would be expected from a reversal by an Oersted field. To obtain switching, the required current density is about 10^7 A/cm^2.

We will also show and discuss the variation of the critical current with the applied magnetic field. This study is of great interest, as the theoretical approaches predict quite different field dependence of the switching current. In Slonczewski's model, the current can be compared to a damping factor (positive or negative, depending on the current sign). To induce reversal, the current has to fight the demagnetizing field, which implies that the applied field has to be compared to the saturated magnetization. On the contrary, in an effective interaction approach, the current acts as a field, which means that the applied field has to be compared to the coercive fields.

Our interpretation is based on the dynamical approach of Slonczewski with a calculation of the current spin polarization in a standard model of the CPP-GMR. The derived critical currents are inversely proportional to this current spin polarization. This means that they are influenced by the thickness of the layer and the spin diffusion lengths in the magnetic and the nonmagnetic layers. Another consequence is their dependence on the magnetic configuration : switching from P to AP is not expected at the same current than switching from AP to P.

Optimizing the parameters of the samples, the critical currents can certainly be reduced and be of interest for application to the switching of submicronic magnetic devices.

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Spin-Polarized Transport in Magnetic Double Barrier Junctions

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A quantum theory of the tunnel magnetoresistance (TMR) in asymmetric magnetic double barrier structures of the form M1/O2/M3/O4/M5 is presented (M and O are the magnetic metal and oxide layer respectively). The evaluation of the current through the double barrier junction is based on the extension of the Kubo formalism to the case of tunnelling. This has been done via the non-local probability using the Green functions technique in the mixed real space-momentum representation. The electron scattering in the metallic layers and the effective mass of the electron in the oxide layers are taking into account. The magnetic double barrier structures are very promising to study fundamental phenomena and for the application in tunnelling magnetic random access memories (MRAM). We have shown that double barrier junctions can be used as a blocking device (diode) in MRAM. We have proposed two concepts which lead to a diode-like behaviour in the I-V characteristics and in TMR of magnetic double barrier junctions. Moreover, the characteristics of this diode are sensitive to the applied magnetic field which makes possible to introduce the concept of magnetically controlled diode. Furthermore, it is shown analytically that the presence of the electron scattering in the middle metallic layers is a necessary condition which has to be taken into account for the calculations of the transistor characteristics when the double barrier junction is considered as a three terminal device. The influence of the random fluctuations of the barrier and the middle metallic layer thickness and of the electron scattering on the diode characteristics and on the quantum well states in the middle metallic layer is investigated.

Perpendicular transport in Fe/Semiconductor heterostructures

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By using the fully relativistic spin-polarized versions of the Screened KKR method and of the Kubo-Greenwood equation the electronic structure, magnetic properties, interlayer exchange coupling and perpendicular electric transport are calculated for Fe/A/Fe heterostructures, with A = Ge, ZnSe, InP. In the case of binary spacer materials particular emphasis is given to the question of termination. It is shown that depending on termination the IEC and the electric transport behave different from each other. The calculation indicate that even for a spacer thickness of 100 Å the magneto-resistance is quite sizeable. The calculated values vary from 20% to 45% depending on termination and material. In the case Ge different spacer structures are studied. It is found that the concentration of vacancies plays a crucial role for the existence of a sizeable magneto-resistance, while the actual structure of the spacer seems to be less important. For all structures the magneto-resistance varies between 35% and 45%, but if the vacancy concentration becomes larger than 10% the magneto-resistance vanishes.

Formation of Weak Ferromagnetism in $Y(Co_{1-x}Al_x)_2$ Compounds: A CPA Study

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The band structure of the substitutionally disordered $Y(Co_{1-x}Al_x)_2$ has been calculated for various concentrations $0 \leq x \leq 0.25$ employing the Coherent Potential Aproximation (CPA) embodied in an all electron TB-LMTO method. Based on these results we provide a new explanation for the weak ferromagnetic moment formation in this compounds. The discussion of the non-spin polarized calculated densities of states is supported by direct evidence of the weak ferromagnetic states for certain lattice constants and Al concentrations. The role of the disorder and the volume effects are disscussed.

Modeling STM tips by single absorbed atoms on W(100) films: 3d and 4d transition metal atoms.

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In order to provide comprehensive data on the electronic structure of realistic STM tips we have studied tungsten (100) films with adsorbed single 3d and 4d transition metal atoms by ab-initio molecular dynamics and full potential methods. Molecular dynamics using ultrasoft pseudo potentials has been used to determine the relaxation of adsorbate and surface layers. Subsequently the electronic structure of the relaxed model-tip has been calculated with an all-electron full potential method. The results suggest that the chemical nature of the tip apex to a high degree determines achievable corrugations and that results for current and corrugation values in a perturbation approach might be considerably improved by including the electronic structure of the tip.

Kerr spectra calculated for multilayer systems

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In the present contribution, we are presenting theoretical Kerr spectra of Co/Pt multilayer systems calculated on a first principles basis including multiple reflections and interferences on the boundaries in–between the layers.

The complex optical conductivity tensor is calculated by means of a contour integration technique, which permits the calculation to be performed at nonzero temperatures and for finite life–time broadening based on the Kubo formula. In combination with the spin–polarized relativistic screened Korringa–Kohn–Rostoker band structure method, this technique provides the most proper first principles calculation mode of the complex optical conductivity tensor in layered systems without using the Kramers–Kronig relations, but accounting on the same footing for both the inter– and the intra–band contributions. The computational accuracy, on the other hand, is permanently controlled by using the Gauss–Konrod quadrature and the recently developed cumulative special–points method.

Magnetic anisotropy of ordered and disordered Mn/Pt multilayers

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The magnetic moments and the anisotropy energy of layered surface compounds formed by $Mn_xPt_{(1-x)}$ ($x \in [0,1]$) on a Pt(111) substrate are calculated by means of the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker (SKKR) method. The disordered binary compositions are modelled within the coherent potential approximation (CPA). Different Mn concentrations at each layer have been considered in order to understand the influence on the magnetic properties of both the chemical environment of the Mn atoms and the segregation of Pt from the bulk. Special emphasis is devoted to the study of the layered sequences $Pt/Mn_xPt_{(1-x)}$, due to the existence of an ordered surface compound of composition $Pt/MnPt_3$.

Magnetic anisotropy of ultrathin Co-films on Cu(111) including relaxation effects

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Magnetic moments and anisotropy energies of thin films of pure Co on a Cu(111) substrate are calculated making use of the fully relativistic spin-polarized screened KKR (SKKR) method. In this *ab-initio* study the influence of layer relaxation and the film-thickness on the magnetic properties of the system is investigated. The number of Co layers was varied from $N = 1$ to $N = 7$ layers and a homogeneous relaxation between $R = -4\%$ and $R = +3\%$ with respect to the Cu bulk lattice constant has been studied. From the calculations an in-plane magnetization for film-thicknesses above four monolayers of Co is predicted for any relaxation. In the case of two and three monolayers a perpendicular orientation of the magnetic moments can be energetically slightly favoured in dependence on the relaxation.

Magnetic properties of adatoms and small clusters on metallic surfaces

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A Green's function embedding technique based on the fully relativistic spin-polarized Screened Korringa-Kohn-Rostoker method is used to calculate the electronic and magnetic properties of Fe, Co and Ni nanostructures deposited on Ag(100). Strongly enhanced spin and orbital moments are obtained for adatoms and for small clusters of Fe and Co. As a consequence, for these clusters considerably larger magnetic anisotropy energies are found than for the corresponding monolayers. In the case of Ni, the occurrence of stable magnetic states turns to be very sensitive on the nanostructure considered. The exchange coupling energy is also investigated for various distances between two adatoms.

Partner Netherlands

The transmission polarization of ferromagnet/superconductor interfaces

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Andreev reflection at an interface between a ferromagnet (FM) and a superconductor (S) has become an attractive technique to measure the spin polarization of magnetic materials. The results of these measurements are interpreted using the so-called BTK model introduced almost twenty years ago which is based on a free-electron model of the conduction electrons and an interface modelled by a delta function with strength Z. In neglecting the complex *d*-bands of transition metal elements, such models are known to neglect important aspects of the physics of electron transport through interfaces; the spin-dependence of the interface transmission plays an essential role in Giant MagnetoResistance. An additional complication is that most FM/S interfaces (such as Co/Pb or Co/Nb) are not epitaxial and difficult to model realistically on an atomic scale. Using a newly developed method based on the TB-LMTO method, we model FM/S interfaces using large lateral supercells, calculate entirely from first-principles the spin polarization of the transmission through Pb/Co and Pb/Cu interfaces and use the results to calculate the conductance above and below the superconducting transition temperature (thus, taking into account the Andreev reflection). This allows us to make a detailed comparison with experiment and discuss the conclusions which can be drawn about the spin-polarization of the ferromagnet.

Theory of spin transport across hetero-interfaces

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Interfaces between ferromagnetic and non-magnetic metals are essential functional elements of magnetoelectronics because of the high spin-selectivity of the electron transmission probabilities. In order to understand and control the spin-injection process, qualitative and quantitative understanding of the electronic structure is important. Interesting novel physics like the spin-current induced torque on the magnetization is also strongly localized to the interface. Within a semiclassical approximation scheme, the characteristics of magnetoelectronic circuits and devices can be expressed in terms of four interface parameters, viz. the conventional spin-up and spin-down conductances and the real and imaginary part of the mixing conductance or spin-torque. The first two are experimentally accessible by transport experiments on magnetic multilayers in the current perpendicular to the plane (CPP) configuration as pioneered by the MSU collaboration. The last two can at least in principle be measured via the angular magnetoresistance of CPP spin valves. We present results for the interface conductances as computed by first principles for specular and disordered interfaces. The results will be compared with available experimental data and the consequences for the physical properties of mesoscopic circuits and devices will be discussed.

Absolute spin-valve effect with superconducting proximity structures

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We investigate spin dependent transport in hybrid superconductor normal-metal ferromagnet (S/N/F) structures under conditions of proximity effect. We demonstrate the feasibility of the absolute spin-valve effect in a certain interval of voltages. We present results for a general magnetic configuration of the ferromagnets involved and for different strengths of the proximity effect.

Ab initio calculations of tunneling magnetoresistance

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Using a recently developed method for calculating transmission matrices from first principles, we study tunneling magnetoresistance focusing our attention on the influence of disorder on the conductance. 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 specular and diffuse scattering can be treated on an equal footing.

Ab – initio electronic structure calculations of correlated systems

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One of the interesting problems in the physics of the strongly correlated electron systems is the development of the local density approximation (LDA) band structure calculation in order to include many-body correlation effects. Here we present a generalization of Exact Muffin–tin Orbitals approach (EMTO) including many-body technique in the frame of recently developed dynamical mean field theory (DMFT). Several test calculations on transition metal and their oxides are presented.

Partner Sweden

Defect induced partial magnetic order in $(Ga_{1-x}Mn_x)As$

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First principles theory and experimental work show that magnetic structures involving disordered local magnetic moments on the Mn atoms in $(Ga_{1-x}Mn_x)As$ lowers the total energy compared to simple ferromagnetic coupling when As defects are considered. Hence

a novel magnetic structure with only partial disorder of local moments is stable for a range of concentrations of As defects. Only by considering this magnetic configuration can one resolve the conspicuous disagreement between calculated and measured magnetic moments in $(Ga_{1-x}Mn_x)As$. A microscopic mechanism for the stabilization of the magnetic structure is suggested. Based on this finding we propose that the saturation magnetisation and critical temperatures of $(Ga_{1-x}Mn_x)As$ should be increased substantially by eliminating or reducing the number of As defects.

Surface Core Level Shift in PdMn systems on Pd(100) by the model of Complete Screening

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Surface and interface core level shifts (CLS) are calculated for an 1 ML Mn/Pd(100) system, and compared to a recent experimental study by A. Sandell *et al.* (in manuscript). The calculations are carried out in the framework of KKR-ASA (CPA), and in some cases compared with the supercell LSGF calculations. Comparison is also made between different models for the core level shift; the initial state model, where the CLS is given directly by the difference of energy eigenvalues for the electrons, and the more complex model of complete screening, which include a relaxation of the core-hole, due to the excited electron (the final state effect). The technique is first applied to a study of CLS for $3d_{5/2}$ electrons in the random bulk alloys CuPd and AgPd. It is shown that for both bulk alloys, as well as for the PdMn system, the model of complete screening gives substantially better agreement with experiment. In the case of Mn/Pd(100) system, we observe that the CLS for an interface Pd atom change sign as compared to the clean Pd(100) surface.

Bulk ordering and surface segregations in the NiPt and NiPd alloys

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A first principles technique for simulations of atomic ordering in a bulk and segregations on surfaces of transition metal alloys has been developed. The technique combines the

screened generalized perturbation method (SGPM) for calculating of effective interatomic interactions in alloys with the Monte Carlo method for deriving equilibrium alloy configuration. The screened generalized perturbation method (SGPM) allows one to take into account both the one-electron and Madelung energy contributions into ordering. A new Monte Carlo method for simulations of surface segregations has been proposed. Using the technique we have obtained the temperature of disorder-order transition in $Ni_{50}Pt_{50}$ as well as short-range order parameters above ordering temperature. The segregation profiles on the low-index surfaces of disordered and ordered NiPt and NiPd have also been calculated.

First principles study of ferromagnet-semiconductor interfaces

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In the context of magnetoelectronics, the knowledge of the interface between a ferromagnet and a semiconductor is necessary. Here we present the results of the structural and magnetic studies of various ferromagnet-semiconductor interfaces viz. Fe/GaAs, Fe/ZnSe, Fe/InAs and Fe/Ge. Calculations have been done with an ab-initio plane-wave pseudopotential code alongwith full geometry optimizations. Various thickness of Fe layers has been considered in order to get a proper understanding of the formation and magnetic properties of the interfaces. We have also studied the effect of different terminations of surfaces and the surface segregation of semiconductor constituents alongwith the effect of surface reconstructions. Lastly, we present some results of the interlayer exchange coupling across semiconducting barriers. The results are in good agreement with the experimental findings.

Partner Hungary

On the Magnetic Structure of γ–FeMn Alloys

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The alloy γ-FeMn is a rare example of a fcc antiferromagnet and, as a consequence, as become a prototype for pinning layer studies in magneto-electronic devices. Whilst it is difficult experimentally to uniquely determine the ground state magnetic structure, first principles calculations based on the KKR-CPA method (Schulthess et al.) point to the non-collinear 3Q structure from amongst three candidate structures [1Q, 2Q and 3Q]. However, because the KKR-CPA method treats disorder within a single site, or mean

field, approximation we are still left with the conceptual problem of how an ordered, non-collinear magnetic state can exist in a compositionally disordered alloy. Here we report the results of first principles calculations of the magnetic structure of γ-FeMn based on large cell models (up to 2048-atoms) of the disordered alloy. The calculations are based on the constrained local moment model and use of first principles spin dynamics to obtain the ground state orientational configuration. Energetically we again find the 3Q-state to be lowest of the three structures studied previously. However, we find the constraining fields, introduced into the theory to maintain a specific orientational configuration, to be non-zero, indicating that even the 3Q-structure is not the ground state. Subsequent optimization of the magnetic configuration using first principles spin dynamics yields a state lower in energy by 2.5 mRy/atom. This new state can be viewed as a relaxed-3Q state in which the individual Fe and Mn site moments are randomly distributed around the ideal 3Q structure.

Theoretical study on non–collinear magnetic structures by means of fully relativistic KKR method

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The magnetic structure of thin films can differ considerably from the magnetic structure of bulk materials. In a previous study we pointed out that a simple classical Heisenberg model with additional magnetic dipole–dipole interaction and uniaxial anisotropy terms can supply non-collinear canted ground states.

In the present study we attempt to describe the magnetic ground states of few atomic layers of magnetic materials from first principle. Analytic expressions have been derived for the first and second derivatives of the band energy with respect of the magnetic orientations in the frame work of the spin–polarized fully relativistic screened KKR method. These derivatives have been also demonstrated in the case of model Bloch–walls in Fe. Using a conjugated gradient technique the magnetic configuration corresponding to the lowest band energy can be easily found. Our formalism also permits the calculation of the low–energy spin–excitations of thin magnetic films.

Magnetic properties and stability of palladium and rhodium nano-clusters

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Ab initio calculation performed for $T = 0K$ shows that in Pd and Rh clusters below a critical size the high surface energy anisotropy stabilizes the icosahedral multiply twinned particle structure against the fcc single crystals. Model structure calculation supports the appearance of ferromagnetic order in Pd clusters with non-crystallographic icosahedral symmetry with a small ($0.11\mu_B$) magnetic moment per atom, while the Rh clusters prooved to be nonmagnetic. These results allow us the interpretation of recent experimental findings [Europhys. Lett., **38**, 195, (1997)] that small free palladium clusters exhibit spontaneous ferromagnetic order.

Partner Czechia

Magnetoresistance effects in disordered bulk alloys by means of the TB-LMTO-CPA method

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The first part of the contribution reviews a recently developed ab initio approach to the interatomic electron transport within the Kubo linear response theory. The approach is based on a systematic neglect of the electron motion inside the atomic (Wigner-Seitz) cells leading thus to velocity operators describing pure intersite hopping.

In the second part, numerical implementation of the formalism within the TB-LMTO-CPA method is described and results of its application to residual resistivity of magnetic bulk transition-metal alloys are presented. Investigated systems include the ferromagnetic Ni-Cu alloys, the disordered local-moment state of the Ni-Mn alloys, and the FeRh-based alloys with atomic long-range order which exhibit large magnetoresistance effects.

Ab initio theory of perpendicular transport in layered magnetic systems

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The current-perpendicular-to-plane (CPP) magnetoresistance of a sample sandwiched by two ideal leads is described at an *ab initio* level. We use the Landauer formulation of the conductance based on surface Green functions as formulated by means of the tight-binding linear muffin-tin orbital method. The formalism is extended to the case of lateral supercells with random arrangements of atoms of two types which in turn allows to deal with ballistic and diffusive transport on equal footing. Applications refer to fcc-based Co/Cu/Co(001) spin valves as well as to multilayers in both the ballistic and diffusive regimes. We will consider in detail the effect of substitutional alloying in spacer and at sample interfaces and, in particular, we will discuss (i) the separation of the ballistic and diffusive parts of the transport, (ii) the separation of the influence of bulk and interface disorders, and (iii) the influence of the order of magnetic and non-magnetic layers on the sample conductance.

Electron correlations in metallic systems

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The electronic and magnetic structure of transition metals with electron correlations between d-electrons is described by a multi-band Hubbard Hamiltonian. The tight-binding linear muffin-tin orbital method is used to construct the one-particle part of the Hamiltonian, while the two-particle part contains suitably parameterized direct and exchange interactions (U and J). The correlation effects are described within the fluctuating-exchange (FLEX) approximation including all electron-electron and electron-hole scatterings in a single channel. The many-body problem is solved in a selfconsistent manner within the dynamical mean-field theory. We assume a single-site character of the one-particle selfenergy. The disorder is treated within the coherent potential approximation. The densities of states and magnetic moments calculated for $3d$ metals and their disordered alloys will be discussed and compared to experimental data.

Mn impurities in GaAs and GaP crystals

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Ground state of Mn in III-V semiconductors still attracts experimental as well as theoretical interest. One unclear problem is the difference between the number of holes in valence band obtained from the transport measurements and proposed from chemical composition. The former is always much smaller than the latter if it is assumed that Mn atom is incorporated substitutionally as an acceptor, creating a hole in the valence band.

We propose an explanation based on the self-compensation property of the Mn impurities: some Mn atoms occupy interstitial rather than most common substitutional positions. The interstitial Mn is expected to be a double donor, i.e. it compensates two Mn acceptors. This mechanism reduces substantially the number of holes in valence band observed in experiment. The presence of interstitial atoms may also be reason for the lattice expansion with increasing content of Mn.

We present spin-polarized FPLAPW electronic structure calculations for a series of geometries in large unit cell approximation. Mn is incorporated either in substitutional, interstitial or both positions. The differences in electronical behavior of substitutional and interstitial Mn supporting our above suggestion are discussed. Presented spectral characteristics show the important role of Mn impurities not only in magnetism, but also in reconstruction of the electronic structure of III-V semiconductors.

Calculation of tensile strength in iron from first principles

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A tensile test in ferromagnetic iron is simulated by ab initio electronic structure calculations using full-potential linearized augmented plane wave method (FLAPW) within the generalized gradient approximation (GGA). The theoretical tensile strength of iron for [001] loading is determined and compared with that of other materials. Behaviour of total energy during the test is explained in terms of symmetry-dictated extrema. The structural and magnetic response of iron to the loading is analyzed in detail.

Spin-orbit coupling and higher-energy phases in Pb along the trigonal deformation path

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Using full-potential linearised augmented plane wave method we have performed total energy calculations along the displacive trigonal deformation path in Pb, which connects continuosly the bcc, simple cubic and fcc structures. Both local density and generalized gradient approximations were employed. The calculated results may be used to predict the lattice parameters of lead overlayers on various (111) substrates. We also studied the influence of spin-orbit coupling on the total energy in Pb along the trigonal deformation path. The elastic constants were calculated with and without the inclusion of the spin-orbit coupling and compared with existing experimental data.

Non–members

Calculated effects of the iron-oxide layer in Fe|FeO|MgO|Fe spin dependent tunneling junctions

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First-principles calculations of the electronic structure and tunneling magnetoconductance of Fe|FeO|MgO|Fe tunneling junctions are compared to those of Fe|MgO|Fe. We find that the iron-oxide layer greatly reduces the tunneling magnetoconductance. This effect is mainly due to the reduced d density of states on the iron site that results from the bonding of iron with oxygen and to the difference in the symmetry of the oxygen p states in the FeO layer and the MgO layer. Additionally, the asymmetry in the band offsets of the two interfaces when the iron-oxide layer is present on one of the interfaces, results in a slanted effective tunneling barrier which affects the decay rates of the tunneling states in the barrier layer.

Ab initio Calculation and Materials Design of Ferromagnetic Semiconductors

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We discuss the materials design to fabricate the transparent and half-metallic ferromagnets in V or Cr-doped ZnO, ZnS, ZnSe and ZnTe based upon *ab initio* electronic structure calculation with the local-spin-density-functional approximation. The electronic structure and the magnetic properties of 3d-transition-metal-atom-doped II-VI compound semiconductors of ZnO, ZnS, ZnSe and ZnTe are systematically calculated using the Korringa-Kohn-Rostoker method with taking into account the substitutional disorder by the coherent potential approximation. It is shown that V or Cr-doped ZnO, ZnS, ZnSe and ZnTe and, Fe-, Co, and Ni-doped ZnO are ferromagnetic without p- or n-type doping treatment. However, Mn-, Fe-, Co- or Ni-doped ZnS, ZnSe and ZnTe are the spin-glass states.

We propose the stabilization mechanism of ferromagnetic state in 3d-transition-metal-atom-doped (3dTM) III-V (GaN, , AlN, InN,GaAs, GaP, GaSb etc.) diluted-magnetic-semiconductors (DMS) based upon *ab initio* electronic structure calculations. Based upon the calculation, we find that the stabilization mechanism of the ferromagnetic state in 3dTM-doped III-V DMSs is due to the Zener's double-exchange mechanism, (not due to the Zener's p-d exchange mechanism), then the magnetic state is determined by the competition between the ferromagnetic double-exchange interaction and the antiferromagnetic super-exchange interaction. We discuss the chemical trends in the stability of ferromagnetism in Mn-doped III-V-based DMSs of (X,Mn)Y (where, X=Al, Ga, In, and Y=N, P, As, Sb, with fixing the Mn concentration at 5%) by changing the covalency, ionicity and p-d hybridization with varying X and Y.

Based upon *ab initio* electronic structure calculation of 3d transition metal doped ZnO with the local-spin-density-functional approximation, we propose the device design for (i) Mn-doped ZnO-based spin-polarized field-effect-transistor (Spin-polarized FET) in which 100% spin-polarized current is controlled by the gate voltage, (ii) ZnO:$Cr_{1-x}Mn_x$-based or ZnO:$Mn_{1-x}Fe_x$-based photo-induced-magnetic memory in which photo-excitation by visible light create the half-metallic ferromagnet and we can detect it using magneto-optical effect by another visible light, and (iii) $Be_{1-x}Zn_xO$:Co-based or $Mg_{1-x}Zn_xO$:Co-based spin-injection device in which we can inject 100% spin-polarized coherent-spin current into the vacuum. We show that *ab initio* electronic structure calculation is useful not only for the materials design but also for devices design for the semiconductor spintronics.

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Introduction to the Dynamical Mean Field Theory of Correlated Systems and its Implementation in Electronic Structure Calculations

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The Dynamical Mean Field Theory (DMFT) has been developed over the past few years for the quantitative study of strongly correlated electron systems. This approach involves a mapping onto a self-consistent quantum impurity problem. Incoherent and quasiparticle processes are treated on equal footing within DMFT. I will review this approach, as well as its early success in providing a detailed theory of the Mott metal-insulator transition. I will also describe the recent extensions of this method in the context of electronic structure calculations of correlated materials (LDA+DMFT), particularly transition metal oxides and f-electron systems.

A first-principles molecular dynamics study of the Fe/GaAs(001) interface

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In this work we investigate the dynamics of the interface atoms by using molecular dynamic technique. The substrate reconstruction as well as the relaxation processes strongly modify the charge transfer and the magnetization profile. We find that the relaxation can, to a large extent, compensate for artificial electronic effects arising from the variation of the volume. We also find a large tendency of As atoms in the As terminated Fe/GaAs(001) interface to diffuse towards the Fe slab. The obtained results provide a unified description of many interface properties like magnetization anisotropy at the interface, magnetic profile, thickness dependence of stress and tetragonal distortions and Schottky barrier height.

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4 News from the TMR2 Network

'Electronic Structure calculations of materials properties and processes for industry and basic science'

Following the positive Midterm review process, the TMR2 network has made the following changes to the EU-contract: To

- extend the network operation into a fifth year (now ending by February 28th, 2003)
- substitute the node MSI (Molecular Simulations Inc. (now Accelrys)) with node ISMANS (Institut Suprieur des Matriaux du Mans, Le Mans, France).
- substitute the node TU-WIEN (Technical University of Vienna) with node UNI-WIEN (University of Wien).

The two node changes are motivated by the movements of the teamleaders of the 'Surfaces' (E. Wimmer) and 'Magnetism' (J. Hafner) sub-projects. The contract extension is motivated both by science and finance. On the financial side it became evident that there is still money available for network activity, while on the scientific side there are still many interesting problems related to the network workplan, which are worth pursuing. In particular the 'Surfaces' subproject has been lagging behind schedule due to the team leaders change of affiliation. Now at ISMANS, E. Wimmer has recently employed two network PostDocs to push the project on Fe-O surfaces in the coming year.

5 News about two new Research Training Networks

In the second round of the fifth framework two research training networks (RTN) with relation to electronic structure of solids and the psi-k community were invited into the final negotiations for financial support. These are entitled

- **'psi-k f-electron'**: Ab-initio Computation of Electronic Properties of f-electron Materials. Coordinator: A. Svane, Århus, Denmark.

  The research of this Network will provide a substantially improved theoretical understanding of the physical properties of materials containing atoms with incompletely filled f-shells.

  The research has two threads:

  a) *the application of existing methodology to specific scientific problems of high current priority, and*

  b) *the development of new methodology for a more accurate description of f-electron systems.*

  The research topics to be tackled under thread **a)** *include investigations of the industrially relevant pigment Ce_2S_3, and the magneto-caloric compounds such as $Gd_5Si_2Ge_2$, both of which will be pursued in close collaboration with industrial collaborators. Further flagship projects include the influence of lanthanide doping on the properties of high temperature superconductors, and the magnetic structures of surfaces of f-electron materials.*

  The major breakthrough envisaged under thread **b)** *is the generation of a computer code, which implements the Dynamical Mean Field Theory for describing fluctuating f-electrons into state-of the art ab-initio electronic structure methodology. This methodology will be applied to calculate the phase diagrams of Pu and Ce, as well as several other rare-earth and actinide elements and compounds. Thus, materials specific studies will be performed of Kondo-lattice systems, heavy fermions and valence-fluctuating systems.*

  There will be seven postdoc positions available which will be announced soon. The institutions involved are University of Aarhus (Axel Svane), Daresbury Laboratory (Walter Temmerman), Rutgers University (Gabi Kotliar), IFW Dresden (Manuel Richter), Katholieke Universiteit Nijmegen (Sasha Lichtenstein), Ecole Normale Superieure Paris (Antoine Georges), Uppsala University (Olle Eriksson), and Materials Design sarl, LeMans (Erich Wimmer).

- **'Exciting'**: First Principles Approach to the Calculation of Optical Properties of Solids. Coordinator: C. Ambrosch-Draxl, Graz, Austria.

The aim of this network is to reliably compute and predict optical properties of solids. To this end the joint effort of seven groups will focus on the description of excited states within density functional. There are three main tasks dealing with **(1)** *fundamental theory,* **(2)** *programme developlment, and* **(3)** *the investigation of a variety of materials.*

The theory part will comprise time-dependent density functional theory (TDDFT) and perturbational methods like GW, electron-hole correlation (BSE) and density matrix approaches. Code developments for different optical processes will be done in different methods.

There will be seven postdoc positions available which will be announced soon. The institutions involved are University of Aarhus (N. E. Christensen), Universite Catholique de Louvain (X. Gonze), FU Berlin (E. K. U. Gross), MPI Halle (W. Hübner), Uppsala University (B. Johansson), INFM Modena (E. Molinari), and University Graz (C. Ambrosch-Draxl).

6 News from the ESF Programme

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

6.1 ESF Workshop/Conference Announcements

6.1.1 EMRS 2002 Spring Meeting: Atomic Scale Materials Design Symposium

European Materials Research Society

EMRS 2002 Spring Meeting

Symposium A

Atomic Scale Materials Design

Congress Center Palais de la Musique et des Congres, Strasbourg, France

June 18-21, 2002

Supported by the Psi-k Network and the European Science Foundation

Deadline for Abstract Submission: January 14, 2002

On-line abstract submissions:

`http://www-emrs.c-strasbourg.fr/EMRS%202002%20Meetings.htm`

Confirmed Invited Speakers:

Rodney BARTLETT (*University of Florida*)
"Large Scale Simulations using Quantum Chemical Forces"

Steven ERWIN (*Naval Research Laboratory*)
"Iron on GaAs"

Claudia FILIPPI (*Universiteit of Leiden*)
"Quantum Monte Carlo Calculations of Hydrogen Adsorption on Si(100)"

Risto NIEMINEN (*Helsinki University of Technology*)
"Defect Modeling in Semiconductors"

Ruben PEREZ (*Universidad Autonoma de Madrid*)
"Mechanical Properties and the Chemical Bond"

Xavier ROZANSKA (*Eindhoven University*)
"Ab-initio Simulations of Catalytic Reactions Inside Zeolites"

Daniel SPISAK (*University of Vienna*)
"Nanostructured Fe-magnets"

Kurt STOKBRO (*Technical University of Denmark*)
"First Principles Modeling of Molecular Electronic Devices"

Arthur VOTER (*Los Alamos National Laboratory*)
"Accelerating Molecular Dynamics"

Symposium Organizers:

Mehdi Djafari-Rouhani, CNRS-LAAS
Mike Finnis, Queen's University Belfast
Jim Greer, NMRC
Juergen Hafner, University of Vienna
Anatoli Korkin, Motorola

Scientific Committee:

G. Gilmer, Bell Labs, USA
H. Goronkin, Motorola, USA
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D. Pettifor, Oxford University, UK
M. Scheffler, Fritz Haber Institute, Germany
T. Vrotsos, Texas Instruments, USA
G. Wachutka, Technische Universitaet Muenchen, Germany

We seek submissions on electronic structure calculations and computational material science applied to:

Microelectronics and Optoelectronics
Nanotechnology and Biotechnology
Chemical Industries

including

Surfaces and interfaces
Molecules and clusters
Catalysis
Biological molecules, macromolecules, polymers
Plasmas, chemical vapor deposition, atomic layer deposition, and materials processing
Nanostructures

We also seek submissions discussing advances in electronic structure theory, which enable new problems to be investigated.

6.1.2 The European Conference on PHYSICS OF MAGNETISM'02

1-5 July, 2002, Poznan, Poland

http://www.ifmpan.poznan.pl/zp2/pm02.html

Chairmen:

Andrzej Jezierski, *Institute of Molecular Physics, Polish Acadmy of Sciences, Poznań*
Roman Micnas, *Institute of Physics, Adam Mickiewicz University, Poznań*

Partially sponsored by ESF Psi-k Programme

The European Conference "Physics of Magnetism'02". The Conference will take place at Poznan (Poland) 1-5 July, 2002. This is the tenth conference, which is a continuation of the previous ones held every 3 years in Poznan since 1975. The Conference is organized jointly by the Institute of Molecular Physics of the Polish Academy of Sciences and the Institute of Physics of the Adam Mickiewicz University in Poznan.

The Conference is meant as an international forum for the presentation and discussion of novel scientific ideas, in a field of broadly understood magnetic phenomena, experimental results and new magnetic materials. A special emphasis will be focused on:

- novel metallic oxides and anomalous magnetoresistive materials;
- low dimensional quantum magnets;
- heavy fermions, fluctuating valence and Kondo systems;
- quantum tunneling and magnetism in nanoscale;
- magnetic multilayers, surfaces, and nanostructures;
- high temperature superconductors;
- electronic structure.

The main objective of the Conference is to bring together scientists and technologists from Western, Central and Eastern European countries involved in research and application of new magnetic materials and high temperature superconductors. The scope of the Conference is quite wide and covers:

high-Tc superconductors, heavy fermions, mixed valence, rare earths and actinides, quasi-1D and -2D magnets, disordered and amorphous magnetic alloys, magnetic semiconductors, nanostructures, electronic structure etc. The plenary talks will be presented by invited distinguished scientists from all over the world. The programme of the 5-days Conference is planned to consist of 25 plenary talks and about 250 oral and poster contributions.

We hope that, just as the previous conferences (PM'93, PM'96 and PM'99), the PM'02 will be a very fruitful meeting stimulating scientific co-operation between scientists from different countries.

7 General Workshop/Conference Announcements

7.1 ESCM2002 Conference

Conference Announcement and Call for Papers:

ESCM2002: Electronic Structure and Computational Magnetism

15-17 July, 2002

Washington, DC

ORGANIZING COMMITTEE:

B.N. Harmon, Ames Laboratory
A.Y. Liu, Georgetown University
D.A. Papaconstantopoulos, Naval Research Laboratory
D.J. Singh, Naval Research Laboratory
G.M. Stocks, Oak Ridge National Laboratory

SCIENTIFIC ADVISORY COMMITTEE:

O.K. Andersen (Germany)	W.H. Butler (U.S.A.)	
A.J. Freeman (U.S.A.)	B.L. Gyorffy (U.K.)	M. Jarrell (U.S.A.)
B. Johansson (Sweden)	M.I. Katsnelson (Russia)	B.M. Klein (U.S.A.)
B. Lengsfield (U.S.A.)	A.I. Lichtenstein (Holland)	A.H. MacDonald (U.S.A.)
I.I. Mazin (U.S.A.)	A.J. Millis (U.S.A.)	T. Oguchi (Japan)
G.A. Sawatzky (Canada)	K. Schwarz (Austria)	W.M. Temmerman (U.K.)

We are pleased to announce the conference, "ESCM2002: Electronic Structure and Computational Magnetism", which will be held July 15-17, 2002 on the campus of Georgetown University. This is the second in the ESCM (following ESCM2000, http://cst-www.nrl.navy.mil/escm2000). Details regarding abstract submission and registration will be posted on the conference web site (http://cmpweb.ameslab.gov/escm2002) in mid-January.

The goal of the conference is to bring together experts and students to discuss the electronic theory of magnetism and magnetic materials as well as couplings from the atomic to the micromagnetic length scale. Some topics of interest are:

* Coupling Length Scales: Atoms to Micromagnetics
Domain wall structure and interactions
Non-Collinear Magnetism
Magnetic anisotropy
Nano-structured magnets
Spin Dynamics
Magnetic Semiconductors
Rare-Earth and Actinide Magnetism
Half-Metals
Molecular Magnets
Magnetic Excitations
Spin-Polarized Transport
Strong Correlations and Magnetism
Magnetism and Superconductivity

We hope to have substantial participation by young scientists. To this end the costs for registration and housing will be very moderate, and additionally we expect to subsidize a number of the student and postdoctoral attendees.

The format will allow plenty of time for discussion. It will consist of a small number of plenary talks by recognized experts in the field, invited talks that will be selected from the contributed abstracts and contributed (poster) sessions.

We look forward to seeing you in Washington this summer.

7.2 EuroConference on "Structure and reactivity of oxide surfaces"

FUNDAMENTAL ASPECTS OF SURFACE SCIENCE

Acquafredda di Maratea, Italy, 1-6 June 2002

http:// www.esf.org/euresco

Chairman: Gianfranco Pacchioni (Universitá Milano Bicocca)

Organizing committee:

Francesc Illas (Universitat de Barcelona, Spain)
Notker Rösch (Technische Universität München, Germany)

Applications Deadline: March, 12 - 2002.

CONTENTS

Oxide surfaces, and metal-ceramic interfaces are relevant in corrosion protection, adhesion, microelectronics, photovoltaic cells, sensors, heterogeneous catalysis, but little is known about their atomistic structure. Thanks to a spectacular development of experimental methods in the last decade, today it is possible to prepare oxide surfaces by applying techniques of epitaxial growth. Data coming from these experiments can be compared with more traditional approaches to the surface chemistry of polycrystalline materials and to ab initio modeling. From the interplay of experiment and theory, significant advances in this area have been achieved. This meeting will cover topics like the structural properties of clean and metal covered oxide surfaces, similarities and differences of single crystals, thin films and polycrystalline materials, adsorption and chemical reactivity, point and extended defects, etc.

SPEAKERS

Charles T. Campbell (*University of Washington, Seattle, WA, USA*)
Hajo Freund (*Fritz-Haber Institut der MPG, Berlin, Germany*)
Elio Giamello (*Universit di Torino, Italy*)
Wayne Goodman (*Texas A&M University, College Station, TX, USA*)
Yashuiro Iwasawa (*University of Tokio, Japan*)
Nicholas M. Harrison (*CCLRC Daresbury Laboratory, Warrington, UK*)
Ueli Heiz (*University of Ulm, Germany*)
Claude R. Henry (*CRMC2-CNRS, Campus de Luminy, Marseille, France*)
Uzi Landman (*Georgia Institute of Technology, Atlanta, GA, USA*)

Falko Netzer (*Karl-Franzens Universität Graz, Austria*)
Claudine Noguera (*Universit de Paris Sud, Orsay, France*)
Jose Rodriguez (*Brookhaven National Laboratory, Upton, NY, USA*)
Matthias Scheffler (*Fritz-Haber Institut der MPG, Berlin, Germany*)
Christof Wöll (*Ruhr-Universität Bochum, Germany*)
Adriano Zecchina (*Universit di Torino, Italy*)

7.3 IBM-NeSC Protein Science Workshop

First Announcement

March 15 and 16, 2002
National e-Science Institute in Edinburgh, UK

On Friday and Saturday, March 15 and 16, 2002, the IBM Blue Gene Protein Science project and the UK National e-Science Center will host the Protein Science Workshop "Blue Gene 2002" to be held at the National e-Science Institute in Edinburgh. The first Blue Gene workshop on Protein folding was held in 2001 at San Diego, California, USA.

The purpose of this workshop is to bring together distinguished scientists whose research is in selected areas of protein science, with emphasis on computational approaches, to establish the status of the research, discuss open issues, reinforce interactions and create new collaborations. The workshop will consist of invited talks divided in three sessions (protein folding, enzymatic reactions and drug design, and systems biology) as well as of contributed posters. Within each session, time will be reserved for informal discussions.

Up-to-date information can be found on

`http://www.zurich.ibm.com/~cur/bg2002/bg2002.html`.

We'll keep updating the program and other details directly on this site. We'll send the second and final announcement by mid February.

Please register and submit your abstract directly by going to the web site above (starting on Monday Jan 7, 2002).

If you have specific questions please do not hesitate to contact either Dr Lindsay Sawyer (l.sawyer@ed.ac.uk) or Dr Wanda Andreoni (and@zurich.ibm.com).

The workshop program committee:

Wanda Andreoni, IBM Research Zurich Research Laboratory
Andrew Coulson, University of Edinburgh
Dietlind Gerloff, University of Edinburgh
Robert S. Germain, IBM Research TJ Watson Research Center
Joseph M. Jasinski, IBM Research TJ Watson Research Center

Anthony D. Kennedy, Maxwell Institute, University of Edinburgh
Anne Kenway, University of Edinburgh
Lindsay Sawyer, University of Edinburgh
Gustavo A. Stolovitzky, IBM Research TJ Watson Research Center

8 General Job Announcements

Postdoctoral Position in Computational Materials Science Group

National Renewable Energy Laboratory
http://www.nrel.gov/cms/

The Computational Materials Science (CMS) Group at the National Renewable Energy Laboratory invites applications for postdoctoral researcher positions to start in the summer or fall of 2002. Applications are accepted now. The positions are for one year, but renewable upon mutual agreement and available funding up to two more years. The research projects are in the areas of theoretical study of electronic structures of photovoltaic materials, defect physics in semiconductors and insulators, and atomic ordering in semiconductor alloys. Experience with first-principles density-functional theory is preferred. The starting salary is US$ 40-52 K/year depending on qualification. The CMS group currently has two senior members (Dr. Su-Huai Wei and Dr. Shengbai Zhang) and four postdoctoral fellows. The group has outstanding computational facilities, an excellent basic-research atmosphere, and is located near the beautiful Rocky Mountains. For more information about the group's research activities, publications and personnel, see http://www.nrel.gov/cms/. Interested candidates should send a curriculum vitae, list of publications and list of three reference letters to

Dr. Su-Huai Wei
Computational Materials Science Group
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado, 80401
swei@nrel.gov

NREL is an equal opportunity/affirmative action employer.

TWO POSTDOCTORAL POSITIONS IN ADSORPTION THEORY

ITALIAN NATIONAL INSTITUTE FOR THE PHYSICS OF MATTER (INFM)

and

ITALIAN MINISTERY FOR UNIVERSITY AND RESEARCH (MURST)

Two postdoctoral positions for research in adsorption theory within two national projects, financed one by the Italian Institute for the Physics of Matter and one by the Italian Ministery for University and Research are available starting early in 2002. The successful applicants will work at the surface physics theory group of Prof. G.P. Brivio at the University of Milano-Bicocca. The key aspect of these projects is the calculation of the electronic properties of selected adsorbate systems. Research will deal both with ground state properties of noble gas atoms, magnetic adsorbates and chemisorbed and physisorbed molecules, and with excited state ones such as Auger spectra of adsorbates. The positions are both for one year with the possibility of extension by 1 or 2 years. Applicants should have experience in first principle electronic structure calculations. The salary is in the range of 13000-15000 Euro per year according to age and experience. For further information, please contact Prof. Gian Paolo Brivio, Dipartimento di Scienza dei Materiali, Universit di Milano Bicocca, via Cozzi 53, 20125 Milano, Italy.

e-mail: gian.paolo.brivio@mater.unimib.it
Tel: (+39)0264485220
Fax: (+39)0264485403

Postdoctoral/Research Associate Positions in Electronic Structure Theory with Alex Zunger

National Renewable Energy Laboratory (NREL)

http://www.sst.nrel.gov

NREL's Solid State Theory Group is looking to fill postdoctoral or research associate positions in the areas of Electronic Structure Theory of (1) nanostructures, (2) alloys, as well as (3) method development. These positions are with Dr. Alex Zunger and extend for 2-3 years starting January-August 2002 Applicants are expected to have a background in solid-state theory. Depending on experience and qualifications, the position could be at the rank of post-doctoral fellow ($40,000 - $53,000 per year) or Research Associate ($52,000 - $65,000 per year). More details about ongoing work in the group, computer facilities, personnel, publications are included in http://www.sst.nrel.gov. Clarification or further details can be obtained via e-mail to azunger@nrel.gov.

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

Dr. Alex Zunger
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401

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

POST-DOCTORAL POSITION

National Institute for Materials Science*

1-2-1 Sengen, Tsukuba-Shi 305-0047, Japan

* Merger of National Research Institute for Metals and National Institute for Research in Inorganic Materials from April, 2001.

Applications are invited for a post-doctoral position funded by New Energy and Industrial Technology Development. The position will start from next April and will last at least for the next Japanese fiscal year and possibly extend to another 2 years. Subject to relevant regulations in the institute, the salary is about 6.5 million Yen per year including various benefits. Business travel will be paid independently. The research subject is on the modeling and simulation of structure and mechanical properties of metal-ceramics interface. The candidate will take part in a joint research project with other institutes and companies. By cooperating closely with research in first-principles and meso-scale and continuum mechanics, he will be asked to construct atomic potentials for the metal and oxide interface and then compute the interface structure and mechanical properties using classical molecular dynamics (MD). He may be stationed at Tsukuba or University of Tokyo. He should have necessary skills and experience in computational materials science; background in material science or related fields and MD computation is preferred.

Please, send inquiries and applications to:

Dr. Liu Yufu
National Institute for Materials Science
1-2-1 Sengen, Tsukuba-Shi 305-0047, Japan
TEL: +81-298-59-2447
FAX: +81-298-59-2401
Email: LIU.Yufu@nims.go.jp

Postdoctoral Position in Electronic Strucutre of Correlated Materials

Rutgers University, Piscataway, USA

We are looking for somebody with experience in electronic structure calculations and with a strong interest in learning and applying new many body techniques to real materials, or somebody with a very strong backround in computational many body theory, with an interested in learning electronic structure. This is an exciting new area of research, which is supported by a strong collaboration with S. Savrasov at NJIT, and many international collaborations. For more information see `http://www.physics.rutgers.edu/~kotliar/postdoc.html`. The position is available immediatly.

Gabriel Kotliar
Professor of Physics
Department of Physics and Astronomy
Serin Physics Laboratory
Rutgers University
136 Frelinghuysen Road
Piscataway
NJ 08854-8019
USA
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Email: kotliar@physics.rutgers.edu
Fax: 732-445-4343

`http://www.physics.rutgers.edu/~kotliar/`

Postdoctoral Position

Electronic Structure Theory

Department of Materials Science and Engineering of the Massachusetts Institute of Technology

A postdoctoral research position in computational materials science/electronic-structure theory is immediately available in the group of Prof Nicola Marzari, in the Department of Materials Science and Engineering of the Massachusetts Institute of Technology.

Experience with first-principles density-functional theory is required. The position is available for up to two years; the salary range is US $36,000 - 40,000, depending on experience.

Detailed informations are available at http://nnn.mit.edu/postdoc.

Postdoctoral Position

Advanced Studies Center, Hewlett-Packard Laboratories

A research position for computational condensed matter physicist is available at HP Labs, Palo Alto. The successful applicant will perform research in condensed matter theory with emphasis on transport in nanoscale structures using first-principles, semi-empirical, and other model approaches. The successful applicant is expected to use the existing and develop new software tools needed for the studies, therefore the candidates with strong computational background (F9x, C) will have an advantage. The position is part of the programme sponsored by DARPA. The interaction with local experimentalists is expected and encouraged for the recruited research fellow. Thebegin appointment will be on a yearly basis with renewals possible for second and possibly third year. HP Labs provides an excellent working environment. The candidate should send a letter of application, CV, and names of three references to A.M. Bratkovsky, Hewlett-Packard Labs, 1501 Page Mill Road, Palo Alto, CA 94304 (Email: alexmb@exch.hpl.hp.com, fax (650)857-7179), who can provide further details about the job.

Postdoctoral Research Position

Materials Properties Group of the Condensed Matter Sector, SISSA, Trieste, Italy

A postdoctoral research position is available in the Materials Properties group

(http://www.sissa.it/cm/research/mp.htm)

of the Condensed Matter Sector at SISSA, Trieste, Italy.

The successful applicant will work on the first-principles theory of gas-surface interaction, with emphasis on the interaction of simple molecules with transition metal surfaces. The research activity will be part of a collaboration with experimental groups in Genova and at the ELETTRA Synchrotron radiation facility in Trieste, funded by the Italian Ministery for the University. The appointment will be on a yearly basis with renewal for a second year.

The successful applicant is expected to use existing software as well to develop new tools needed for the studies, therefore the candidates with strong computational background will have an advantage. Familiarity with ab-initio density-functional methods is essential.

Candidates should send a CV, together with names and contact information for 2-3 references, to degironc@sissa.it as soon as possible. Consideration of candidates will begin immediately and continue until the position is filled.

Lectureship in Computational Physics

University of Warwick, U.K.

This appointment is associated with the University's newly created Centre for Scientific Computing and is intended to advance computational physics research in one of the Department's relevant areas, namely: Theoretical Physics, Space and Astrophysics, Condensed Matter Physics, Surface Science, Semiconductor Physics, or Structural & Materials Science. This is a permanent post on the Lecturer B scale, available from 1/10/02.

For further details please go to http://jobs.ac.uk/jobfiles/AC1325.html.

Research Position

Condensed Matter Theory Group, Physics Department Cagliari University, Cagliari, Sardinia, Italy

A research contract, starting date approximately May-June 2002, is available in the Computational Condensed Matter Theory Group at the Physics Department of Cagliari University, Cagliari, Sardinia, Italy. The succesful applicant will work in the sub-group of Prof. Vincenzo Fiorentini.

Duration: 24 months.

Starting date: negotiable, around May 2002.

Net salary: ∼1050-1100 euro/month, possible integration negotiable for non-italian applicants. Reasonable travel money is available.

Topic: first-principles study of energetics and electronic structure of InGaAsN alloys containing hydrogen.

Techniques: LDA/GGA DFT using ultrasoft potentials or PAW.

Requirements: degree in physics, chemistry, materials science (e.g. Italian Laurea, German Diplom, US Master). A PhD is obviously a plus. Preference is given to people with previous experience in ab initio calculations on materials, and/or computational physics at large.

Appointment procedure: there is a public selection. Terms for application are being set at the moment, presumably between approximately 1 and 30 March. Selection will follow shortly so that the position could be taken in May.

For more info see Contact, below.

Environment: Workplace in a very modern building. Good computational facilities available. CCMTG is a composite and lively group of comparatively young researchers, including several PhD and laurea students, and the working atmosphere is pleasant.

Contact:

Prof. Dr. Vincenzo Fiorentini
Dipartimento di Fisica
Universitá di Cagliari
Cittadella Universitaria
09042 MONSERRATO (CA), Italy
phone +39 070 675 4912
fax +39 070 510171
e-mail vincenzo.fiorentini@dsf.unica.it

More comments:

The salary is typical for a junior of this level in Italy. For a single, it makes for reasonable living in Sardinia, which is relatively inexpensive to live in. Cagliari is a pleasant city by the sea, with a gorgeous "in-town" beach. Climate is mild (absolute night low $\sim$5 C in December, absolute day high $\sim$36 to 40 C, but windy, in August). Sardinia is probably the largest remaining wilderness area in western Europe, and a world-wide acclaimed sea resort. Local cuisine is intriguing to say the least.

9 Abstracts

5f Resonant Photoemission from Plutonium

J. Terry, R.K. Schulze, J.D. Farr, T. Zocco
Los Alamos National Laboratory, Los Alamos NM
K. Heinzelman, E. Rotenberg, D.K. Shuh
Lawrence Berkeley National Laboratory, Berkeley CA
G. van der Laan
Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK
D.A. Arena, J.G. Tobin
Lawrence Livermore National Laboratory, Livermore CA

Abstract

Experimental resonant photoemission (ResPes) results for α-Pu and δ-Pu bulk samples are presented and compared to the results of an atomic model calculation. Both Pu samples exhibit limited agreement with the atomic calculations. As shown, α-Pu appears to have more 5f valence band delocalization than δ-Pu. Evidence of an enhanced sensitivity to surface corruption, by using synchrotron radiation as the excitation, is presented.

(Surf. Sci. Lett. **499**, 141-147 (2002); February issue)
Contact person: g.vanderlaan@dl.ac.uk

The LDA+DMFT Approach to Materials with Strong Electronic Correlations

K. Held
Physics Department, Princeton University, Princeton, NJ 08544, USA
I. A. Nekrasov and V. I. Anisimov
Institute of Metal Physics, Russian Academy of Sciences-Ural Division, Yekaterinburg GSP-170, Russia
G. Keller, V. Eyert, T. Pruschke, and D. Vollhardt
Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany
N. Blümer
Institute for Physics, Johannes Gutenberg University, D-55099 Mainz, Germany
A. K. McMahan
Lawrence Livermore National Laboratory, University of California, Livermore, CA 94550, USA
R. T. Scalettar
Physics Department, University of California, Davis, CA 95616, USA

Abstract

LDA+DMFT is a novel computational technique for *ab initio* investigations of real materials with strongly correlated electrons, such as transition metals and their oxides. It combines the strength of conventional band structure theory in the local density approximation (LDA) with a modern many-body approach, the dynamical mean-field theory (DMFT). In the last few years LDA+DMFT has proved to be a powerful tool for the realistic modeling of strongly correlated electronic systems. In this paper the basic ideas and the set-up of the LDA+DMFT(X) approach, where X is the method used to solve the DMFT equations, are discussed. Results obtained with X=QMC (quantum Monte Carlo) and X=NCA (non-crossing approximation) are presented and compared. By means of the model system $La_{1-x}Sr_xTiO_3$ we show that the method X matters qualitatively and quantitatively. Furthermore, we discuss recent results on the Mott-Hubbard metal-insulator transition in the transition metal oxide V_2O_3 and the α-γ transition in the 4f-electron system Ce.

(Submitted to: Proceedings of the Winter School on "Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms", February 25 - March 1, 2002, Rolduc/Kerkrade (NL), organized by the John von Neumann Institute of Computing at the Forschungszentrum Juelich)
Latex-file available from http://xxx.lanl.gov/abs/cond-mat/0112079 or kheld@feynman.princeton.edu

Exchange coupling in $CaMnO_3$ and $LaMnO_3$: configuration interaction and the coupling mechanism

M. Nicastro and C.H. Patterson
Department of Physics and Centre for Scientific Computation, University of Dublin, Trinity College, Dublin 2, Ireland

Abstract

The equilibrium structure and exchange constants of $CaMnO_3$ and $LaMnO_3$ have been investigated using total energy unrestricted Hartree-Fock (UHF) and localised orbital configuration interaction (CI) calculations on the bulk compounds and $Mn_2O_{11}^{14-}$ and $Mn_2O_{11}^{16-}$ clusters. The predicted structure and exchange constants for $CaMnO_3$ are in reasonable agreement with estimates based on its Néel temperature. A series of calculations on $LaMnO_3$ in the cubic perovskite structure shows that a Hamiltonian with independent orbital ordering and exchange terms accounts for the total energies of cubic $LaMnO_3$ with various spin and orbital orderings. Computed exchange constants depend on orbital ordering. Exchange contributions to the total energy vary between -20 and 20 meV per Mn ion, differences in orbital ordering energy vary between 3 and 100 meV and a Jahn-Teller distortion results in an energy reduction of around 300 meV. The lattice constant of the lowest energy cubic perovskite structure (3.953 Å) is in good agreement with the lattice constant of the high temperature 'cubic' phase of $LaMnO_3$ (3.947 Å). The total energy of *Pnma* $LaMnO_3$ was minimised by varying lattice parameters and seven internal coordinates and a structure 194 meV per Mn ion below that of a structure determined by neutron diffraction was found. This optimised structure is nearly isoenergetic with a cubic perovskite structure with a 5 percent Jahn-Teller distortion. UHF calculations tend to underestimate exchange constants in $LaMnO_3$, but have the correct sign when compared with values obtained by neutron scattering; exchange constants obtained from CI calculations are in good agreement with neutron scattering data provided the Madelung potential of the cluster is appropriate. Cluster CI calculations reveal a strong dependence of exchange constants on Mn d e_g orbital populations in both compounds. CI wave functions are analysed in order to determine which exchange processes are important in exchange coupling in $CaMnO_3$ and $LaMnO_3$.

(Submitted to Phys. Rev. B)
Available at: cond-mat/0111536
Contact person: Charles H. Patterson (Charles.Patterson@tcd.ie)

True direct gap absorption in Germanium quantum films

Alexander N. Kholod[1], Stefano Ossicini[2], V. E. Borisenko[3], and F. Arnaud d'Avitaya[1]
[1]*Centre de Recherche sur les Mécanismes de la Croissance Cristalline,*
Campus de Luminy - Case 913, 13288 Marseille cedex 9, France
[2]*Istituto Nazionale per la Fisica della Materia*
and Dipartimento di Scienze e Metodi dell'Ingegneria,
Università di Modena e Reggio Emilia,
Via Allegri 13, 42100 Reggio Emilia, Italy
[3]*Belarusian State University of Informatics and Radioelectronics,*
P. Browka 6, 220013 Minsk, Belarus

Abstract

In this paper we provide strong evidence of direct gap absorption in Germanium nanostructured films. By performing first-principle calculations of the optical spectra for the three main low-index orientations we show that due to wavefunctions localization both in real and in reciprocal space the Ge(100) quantum films are, in particular, good candidates for the visible photoluminescence observation.

(Physical Review B, in print, March 2002)
Contact person: Stefano Ossicini (ossicini.stefano@unimo.it)

First-principles study of Pd-V surface alloys: I. Electronic structure of clean surfaces

Robin Hirschl and Jürgen Hafner
Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

Abstract

We investigate the influence of vanadium impurities on the geometric and electronic properties of palladium (111) surfaces using ab-initio density-functional calculations. Our calculations are based on projector augmented wave (PAW) potentials in a plane wave basis set and the Perdew-Wang generalised gradient approximation (GGA) for the exchange-correlation functional. Single layer vanadium concentrations range from $c = \frac{1}{9}$ to $c = 1$ in the surface and subsurface layers. The surface is simulated by repeated slabs consisting of four to eight layers of metal and separated by several layers of vacuum. Impurities are introduced on one side of the slab only where the atoms of the topmost layers are allowed to fully relax. Regarding the electronic structure we investigate the local and partial densities of states (LDOS and PDOS respectively) of the surface atoms of different alloys as well as the LDOS of vanadium. The local effects of alloying on the d-bands of the neighbouring atoms are discussed. Finally we examine surface states of highly concentrated Pd/V surface- and subsurface-alloys. The findings are a first step towards the understanding of the chemical reactivity of surface alloys consisting of a late and an early transition metal.

(**A**) Surf. Sci., 498, 21 (2002))
Contact person: Robin Hirschl (robin.hirschl@univie.ac.at)

First-principles study of Pd-V surface alloys: II. Chemical reactivity

Robin Hirschl and Jürgen Hafner
Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

Abstract

Impurities in transition metal surfaces are known to modify the chemical reactivity of those surfaces. We have previously shown that vanadium in and under Pd (111) surfaces alters the electronic structure of the surface atoms considerably (R. Hirschl and J. Hafner, preceding article). In this work we investigate the changes in the chemical properties of Pd (111) surfaces after alloying with sub-monolayer amounts of V using CO as a test adsorbate. We have performed ab-initio density functional theory (DFT) calculations based on a plane wave basis set and projector augmented wave (PAW) pseudopotentials. The influence of using two different exchange-correlation functionals is studied. We investigate the local adsorption energies and geometries on different alloy surfaces as compared to the pure Pd surface, followed by a detailed analysis of the local and partial density of states of the surface and adsorbate atoms and their electronic interaction. Local adsorption properties can be understood in terms of the changes in the d-band structure through alloying. Our results are discussed in the context of experiments and investigations of other binary transition metal surfaces.

(**B**) Surf. Sci., 498, 37 (2002))
Contact person: Robin Hirschl (robin.hirschl@univie.ac.at)

Magnetism and electronic structure of hcp Gd and the Gd(0001) surface

Ph Kurz[1], G Bihlmayer[1] and S. Blügel[2]
[1] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[2] *Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück, Germany*

Abstract

The localized $4f$ states of Gd represent a challenge for first-principle theory. Our calculations support previous findings that within the local density approximation (LDA) the itinerancy of the $4f$ states is overestimated. In particular, the large density of states at the Fermi energy due to the minority $4f$ electrons is unphysical, and our results show that this is the origin of the incorrect prediction of the antiferromagnetic ground state for hcp Gd by many LDA and generalized gradient approximation (GGA) calculations. We show that different methods of removing these states from the region close to the Fermi energy, e.g. the treatment of the $4f$ electrons as localized core electrons or by using the LDA+U formalism, lead to the prediction of the correct ferromagnetic ground state for the bulk and a ferromagnetically coupled surface layer on the (0001) surface. With these methods ground-state properties like the magnetic moment, the equilibrium lattice constant and surface relaxations can be determined in good agreement with experiment. The energetic position of the surface states of the Gd(0001) surface are compared to experimental data.

(Submitted to J. Phys.: condensed matter)
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Structure and energetics of Cu(100) vicinal surfaces

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Abstract

The multilayer surface relaxations of the Cu(100) vicinals are investigated using a first-principles local density technique. In agreement with the low-energy electron diffraction data for (115) and (117) surfaces we find a large inward relaxation of the step atoms and an about -9% reduction of step heights rather independency of the terrace width. For the further layers we predict the interlayer contraction/expansion trends correctly but the calculated values are too high compared with experiments. From the extracted surface energies and step formation energies of $(11n)$ and $(10n)$ surfaces we conclude formation of distorted octahedral Cu islands on Cu(100) with the longer edges along the $\langle 110 \rangle$ direction.

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http://cms.mpi.univie.ac.at/spisak/publications.html

Shear instability of γ-Fe in bulk and in ultrathin films

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Abstract

Using *ab-initio* local-spin-density calculations we demonstrate that along the Bain path describing the transformation of face-centered-cubic (fcc) γ-Fe into body-centered-cubic (bcc) α-Fe, tetragonal Fe is unstable against monoclinic shear deformations producing a nearly-bcc structure. In the limit of a monolayer adsorbed on a fcc substrate, the epitaxial constraint suppresses the shear instability, but in ultrathin films with three to six monolayers a striped pattern of near-bcc domains develops, confirming recent observations by scanning tunneling microscopy. A strong correlation between the shear instability and the magnetic state is reported.

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On the oxygen-driven magnetization reorientation in Fe(001) bilayer

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Abstract

Experimentally, very small oxygen doses at Fe bilayer grown at Ag(001) change the magnetization direction from perpendicular to in-plane (J. Chen et al., Phys. Rev. B 45 (1992) 3636). We make an attempt to analyze our previous semi-empirical tight-binding model (Š. Pick et al., Phys. Rev. B **63** (2001) 205427). For low oxygen coverage we derive, however, only very small magnetic anisotropy energy changes. Nevertheless, we find indications of the tendency to surface-subsurface antiferromagnetic coupling induced by oxygen and changing markedly the magnetic anisotropy. Another possibility to explain the effect is a preferred oxygen adsorption at specific sites leading to high-coverage regions at the surface.

(To appear in Solid State Comm.)
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First-principles study of nucleation, growth, and interface structure of Fe/GaAs

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Abstract

We use density-functional theory to describe the initial stages of Fe film growth on GaAs(001), focusing on the interplay between chemistry and magnetism at the interface. Four features appear to be generic: (1) At submonolayer coverages, a strong chemical interaction between Fe and substrate atoms leads to substitutional adsorption and intermixing. (2) Between one and two monolayers, a crossover occurs from a preference for intermixed interfaces to more abrupt interfaces. (3) For complete films of any thickness, both Ga- and As-adlayers act as surfactants, dramatically stabilizing the growing films. (4) During the first few monolayers of growth, Ga or As atoms are likely to be liberated from the interface and diffuse to the Fe film surface. Magnetism plays an important auxiliary role for these processes, even in the dilute limit of atomic adsorption. Most of the films exhibit ferromagnetic order even at half-monolayer coverage, while certain adlayer-capped films show a slight preference for antiferromagnetic order.

(submitted to: Phys. Rev. B)
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The role of sub-surface oxygen in oxide formation at transition metal surfaces

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Abstract

We present a density-functional theory trend study addressing the incorporation of oxygen into the basal plane of the late 4*d* transition metals (TM) from Ru to Ag. Occupation of sub-surface sites is always connected with a significant distortion of the host lattice, rendering it initially less favorable than on-surface chemisorption. Penetration only starts after a critical coverage Θ_c, which is lower for the softer metals towards the right of the TM series. The computed Θ_c are found to be very similar to those, above which the bulk oxide phase becomes thermodynamically more stable, thus suggesting that the initial incorporation of oxygen actuates the formation of a surface oxide on transition metals.

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Adsorption of Xe atoms on metal surfaces: New insights from first-principles calculations

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Abstract

The adsorption of rare gases on metal surfaces serve as the paradigm of weak adsorption where it is typically assumed that the adsorbate occupies maximally coordinated hollow sites. Density functional theory calculations using the full–potential linearized augmented plane wave method for Xe on Ti(0001), Cu(111), Pd(111), and Pt(111), show, however, that Xe prefers low–coordination top sites in *all* cases. We identify the importance of polarization, site–dependent Pauli repulsion, and covalency in actuating the site preference and the nature of the interaction between rare-gas atoms and metal surfaces.

(submitted to: Phys. Rev. Lett.)
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What density-functional theory can tell about the spin-density wave in Cr

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Abstract

The energy-vs-volume curve of the spin-density-wave (SDW) in bcc Cr is calculated with the DFT/FLAPW-method using the Generalized Gradient Approximation (GGA). The predicted ground state is not the SDW, in contrast to experiment, and in contrast to an earlier FLAPW calculation. A conjecture is formulated that the widely varying results of LDA and GGA – and of different solution methods – can be scaled by the size of the calculated moment. As a consequence, experimentally relevant properties of the SDW can be calculated by tuning the moment. The implications of these results for the ability of DFT to describe Cr are discussed.

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Ab-initio study of $5f$ localization-delocalization transition from UPd_3 to UPt_3

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Abstract

The electronic structures of URh_3, UPd_3, UPt_3 and UAu_3 are calculated with the self-interaction corrected local-spin-density approximation. We find that only in URh_3 the f-electrons are fully delocalized. UPt_3 has one f-electron localized at each U site, whilst a localized f^2 configuration of the U-ion is found for UPd_3. Upon pressure, UPd_3 will become very similar to UPt_3, and exhibit heavy-fermion behaviour. We predict that in UAu_3 there exists a mixed localized-delocalized f-electron manifold.

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Electronic structure of Pu monochalcogenides and monopnictides

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Abstract

The electronic and magnetic properties of Pu monopnictides and monochalcogenides, PuX (X=N, P, As, Sb, Bi, O, S , Se, Te, Po), are studied using the $ab-initio$ self-interaction-corrected local spin-density approximation. This approach allows for an integer number of f-states to be localized, while the remaining f-electron degrees of freedom are available for band formation. By varying the relative proportions of localized and delocalized f-states, the energetically most favourable (groundstate) configuration can be established. We show that the experimental data can be interpreted in terms of the coexistence of both localized and delocalized f-states.

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10 Available Free Software

Announcement

Ab-initio Molecular Dynamics Program

The CPMD program (Ab-initio Molecular Dynamics Program, developed by J. Hutter, M. Parrinello et al., copyright IBM Corp and MPI Stuttgart) is now available directly on the web (source code in its latest version 3.5) at http://www.cpmd.org.

Any non-profit organization can obtain a free licence there.

11 SCIENTIFIC HIGHLIGHT OF THE MONTH

OPTIMIZING STRUCTURE FOR LARGER, FINITE SYSTEMS

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ABSTRACT

The problems related to the calculation of structure of larger, finite systems are discussed in detail. In particular, it is emphasized *i*) that a complete search in the multidimensional structure space for a given system is without reach for any but the absolutely smallest systems, *ii*) that systematic studies of more systems without severe assumptions about their structure not are possible with current parameter-free electronic-structure methods, and *iii*) that one has to rely on different kinds of 'dirty tricks' in order to calculate the properties of interest. With the embedded-atom method combined with an '*aufbau/abbau*' approach (described in the text) we study structural and energetical properties of metal clusters, whereas for semiconductor nanoparticles we use a tight-binding method in combination with the assumption that their structure can be derived from the wurtzite or zincblende crystal structure. Finally, we study the properties of a series of Ti_mC_n metcars for which we apply a genetic algorithm in the structure optimization in combination with the tight-binding method for the electronic-structure calculation.

1. INTRODUCTION

The problems we shall address in this paper may be best described through an example taken from some recent experimental studies at the University of Konstanz in Germany.

About 10 years ago the group around Castleman in Pennsylvania produced metal-containing carbon clusters M_mC_n. In mass abundance spectra they observed a peak for $(m,n) = (8,12)$ with M being Ti [1], suggesting that this cluster was particularly stable. They proposed a cage-like structure of cubic T_h symmetry with 12 five-membered rings, each containing two metal and three carbon atoms. Thus, the topology is as that of the smallest possible fullerene molecule C_{20} but containing metal atoms. An alternative description of the structure is to consider it as formed by a cube of the eight metal atoms. The 12 carbon atoms forms six C_2 dimers that are placed symmetrically above the sides of the cube with the C–C bonds parallel to the edges. Later, theoretical studies – first of all by Dance [2] — suggested that the structure had tetragonal T_d symmetry. Compared with the T_h symmetry, the C_2 dimers are for the T_d symmetry lying parallel to the diagonals of the six sides of the cube of the eight metal atoms and, in addition, the cube becomes somewhat distorted. First recently, theoretical and experimental studies agree that the tetragonal structure is the correct one (see, e.g., [3]). In the meantime it has been found that also for other metals (e.g., Hf, Zr, V) those so-called metallocarbohedrenes or metcars can be formed, and even metcars with more different types of metals have been produced. However, whether they occur in significant amounts depend strongly on the experimental conditions, suggesting that kinetic effects play a significant role in their production.

In order to study the properties of the Ti-based material further, the group around Ganteför in Konstanz decided to study a whole class of M_mC_n clusters with different values of (m,n) centered around $(m,n) = (8,12)$ [4]. Using two different sources, Ti and C atoms were produced that subsequently were allowed to form the clusters mentioned above. After ionization, a magnetic field could be used to mass-separate the clusters and, finally, photoelectron spectra could be recorded for these mass-selected clusters. Accompanying theoretical studies would then be very useful as a support for the interpretation of the experimental results.

As one of the clusters of the experiments let us choose Ti_6C_{10}, i.e., $(m,n) = (6,10)$, whose structure is absolutely unknown. One *may* consider it as been formed by removing two carbon and two titanium atoms from the more famous $(m,n) = (8,12)$ cluster, but the first question is then: which four atoms shall be removed? Starting with the two proposed structures (i.e., those of T_h and T_d symmetry) for the $(m,n) = (8,12)$ cluster mentioned above we tried this strategy (using a computational method that will be described below) but obtained a new structure in each attempt. The simplest approach would then be to choose the structure of the lowest total energy. However, it has to be remembered that the experiment is performed in a completely different way: instead of starting with the larger $(m,n) = (8,12)$ cluster and from that removing some atoms, the $(m,n) = (6,10)$ cluster is formed from essentially isolated atoms and, therefore, it is not at all given that its structure has any resemblance to that of the $(m,n) = (8,12)$ cluster.

Thus, the first problem in this case is that we have essentially no information about the structure of the system of interest except for its composition but want nevertheless to calculate some of its properties. The second problem is that finite systems of the type A_N have a very rapidly growing

N	No. of structures
7	4
8	8
9	21
10	64
11	152
12	464
13	1328

Table 1: *No. of metastable structures for Lennard-Jones-Clusters LJ_N as a function of N. The results are from [5].*

number of metastable structures as a function of N. As a simple illustration we may consider N identical particles interacting via Lennard-Jones potentials. This system is so simple that it allows for exhaustive studies of the total-energy surface. Tsai and Jordan [5] have performed such studies and in Table 1 we show their results for the number of metastable structures as a function of N. It should be obvious that this number grows rapidly with N.

These problems become even more significant when one wants to study the semiconductor or metal nanoparticles that are of large experimental interest currently. For these the precise composition is often not known and, instead, one has often a certain size-distribution. Moreover, their diameters lie typically in the range 1–100 nm, meaning that the number of atoms per particle is from 100s to several 10 000s.

Studying such systems theoretically with electronic-structure methods one has therefore to be very precise in identifying which questions one attempts to address. For instance, when the so-called magic numbers (the values of N for which the clusters are particularly stable) are sought, it is important to have a good estimate of the lowest total energy for a given value of N, but it may not be necessary to identify the global total-energy minimum. On the other hand, for optical properties or the electron density of either some selected or of all orbitals a good approximation to the structure of the global total-energy minimum should be used, although the structure may not have to be that of a local or the global total-energy minimum. For vibrational properties it may be crucial to have identified the global total-energy minimum.

In the present contribution we shall describe some of the methods we are using in addressing these issues. Due to the size and low symmetry of the systems of our interest and to the large number of structures that have to be studied, we do not consider it possible to apply parameter-free first-principles electronic-structure methods but use approximate methods. For the sake of completeness these methods shall be described briefly in Sec. 2. Subsequently, we shall study different properties of elemental metal clusters in Sec. 3 and of semiconductor nanoparticles in Sec. 4. In Sec. 5 we shall return to the metcars, and a brief resumé is offered in Sec. 6.

2. ELECTRONIC-STRUCTURE METHODS

We use two parameterized methods in our studies of the properties of the nanoparticles.

According to conventional wisdom, the electrons in metallic systems are delocalized and, therefore, less sensitive to the precise positions of the nuclei. For metallic nanoparticles we use, of this reason, the embedded-atom method of Daw and Baskes [6, 7, 8, 9]. The basic idea behind this method is to consider each atom of a metal as an impurity embedded in a host of the rest of the atoms. This provides one contribution to the total energy of the system of interest. The other contribution comes from the interactions between the atoms which is written as a sum of pair potentials. Accordingly, the total energy has the following form

$$E_{\rm tot} = \sum_i F_i(\rho_i^h) + \frac{1}{2}\sum_{i\neq j}\phi_{ij}(R_{ij}). \tag{1}$$

Here, ρ_i^h is the electron density felt by the ith atom but coming from the other atoms. In principle, this density is structured but as a simplification we simply take the value at the site of the nucleus $\vec{R}_i$ of the superposition of the atomic electron densities from the other atoms,

$$\rho_i^h = \sum_{j\neq i}\rho_j^a(R_{ij}) \tag{2}$$

with

$$R_{ij} = |\vec{R}_i - \vec{R}_j|. \tag{3}$$

Using this method requires information on the embedding functions F_i, the pair interactions ϕ_{ij}, and the atomic electron densities ρ_j^a. The latter have been obtained from Hartree-Fock calculations, whereas the former have been specified semiempirically using a combination of theoretical and experimental information on various finite and infinite systems.

For systems with directional covalent bonds it is important to include a precise description of the electronic orbitals and, accordingly, the embedded-atom method is not applicable here. Instead, we use a parameterized density-functional method [10, 11, 12, 13]. With this method the binding energy is approximated as

$$E_B = \sum_i \epsilon_i - \sum_j\sum_{m_j}\epsilon_{jm_j}^a + \frac{1}{2}\sum_{j\neq k}U_{jk}(R_{jk}). \tag{4}$$

Here, $\epsilon_{jm_j}^a$ is the free-atom single-particle energy of the m_jth orbital of the jth atom, whereas ϵ_i is the single-particle energy of the ith orbital of the system of interest. The latter are obtained from the Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2 + V_{\rm eff}(\vec{r})\right]\psi_i(\vec{r}) = \epsilon_i\psi_i(\vec{r}). \tag{5}$$

The solutions ψ_i are expanded in a set of atom-centered orbitals

$$\psi_i(\vec{r}) = \sum_p c_{ip}\phi_p(\vec{r}) \tag{6}$$

with p being a compound index that describes the site, the radial dependence, and the angular dependence of the basis function ϕ_p.

The potential $V_{\rm eff}$ of Eq. (5) is approximated through a superposition of free-atom potentials,

$$V_{\rm eff}(\vec{r}) = \sum_j V_j^a(|\vec{r} - \vec{R}_j|), \tag{7}$$

and it is assumed that the matrix elements $\langle\phi_p|V_j^a|\phi_q\rangle$ only then are non-vanishing when at least one of the functions ϕ_p and ϕ_q is centered on $\vec{R}_j$.

With these approximations the Hamilton and overlap matrix elements can be calculated once and for all as a function of interatomic distance through calculations on diatomic molecules once the basis functions have been specified (we use Slater-type orbitals). Finally, the pair potentials U_{jk} of Eq. (4) are obtained by requiring that results of parameter-free density-functional calculations on the diatomics are reproduced accurately.

3. ELEMENTAL METAL CLUSTERS

Metal clusters M_N with M being a simple metal like Na, K, Rb, Cs have attracted considerable attention during the last two decades since the discovery of so-called magic numbers (for reviews, see [14, 15]), i.e., values of N for which the clusters are particularly stable. These experimental findings can be explained by a simple shell-filling argument: Considering a spherical jellium and focusing only on the valence electrons, these will occupy orbitals of s, p, d, $\cdots$ symmetry, and for those values of N where these shells are filled a particularly stable system is obtained. These values match those found in experiment.

However, the jellium model represents a simplification that may not be justified for any other metal clusters than those of the simple metals. In addition, for clusters of transition metals it is not obvious how many electrons per atom should be considered as valence electrons. Instead, the embedded-atom method provides a more accurate description (including that of the nuclear positions, which is lacking within the jellium model) although it can be argued that in particular for $3d$ transition metals the approximations behind this method may be inadequate. Despite these considerations we have chosen to use this method for transition-metal clusters, since its simplification allows for the calculation of the total energy for *very* many structures as will be needed for a largely unbiased systematic study of energetical and structural properties of these clusters.

The identification of the magic numbers for these clusters requires good estimates of the lowest total energy for a given N. Experimental information can not be used in determining relevant structures (for a more detailed discussion, see [16]) and, therefore, we need an approach that gives good estimates of the structures and total energies of the global total-energy minimum. We have used the following strategy that partly has been devised as a simple means of simulating an atom-by-atom growth process.

1. For a given N we consider of the order of 500–1000 random start geometries. Close local-energy minima for these are found using a quasi-Newton approach.

2. The structure of the lowest total energy is disturbed by moving randomly a part of the atoms. This is repeated some 300–500 times and the thereby resulting lowest-total-energy structure is kept.

3. These two steps are repeated for a cluster with $N+M$ atoms, where we have found empirically that $M \simeq 5-10$ is useful.

4. Starting with the structure of N atoms we add one atom randomly to the cluster and the

structure is optimized. This is done in total some 300–500 times and leads to a structure for the cluster with $N + 1$ atoms.

5. Step 4 is repeated until the cluster with $N + M$ atoms is obtained.

6. In parallel to the steps 4 and 5, one atom is removed from the cluster with $N + M$ atoms that was found in step 3 and determine the closest total-energy-minimum structure. This is done for each of the $N + M$ atoms one by one and leads to a structure for the cluster with $N + M - 1$ atoms.

7. Step 6 is repeated until the cluster with N atoms is obtained.

8. In total these calculations lead to two sets of optimized structures with the number of atoms ranging from N to $N + M$. Only if no new structures with lower total energies are generated, it is assumed that the structures of the global-total-energy minima have been identified.

We would like to stress that our '*aufbau/abbau*' approach does not guarantee that the global total-energy minima have been identified. Only a complete information about the total-energy surface in the $(3N - 6)$-dimensional space can guarantee this, but this information is without reach for any but the absolutely smallest values of N.

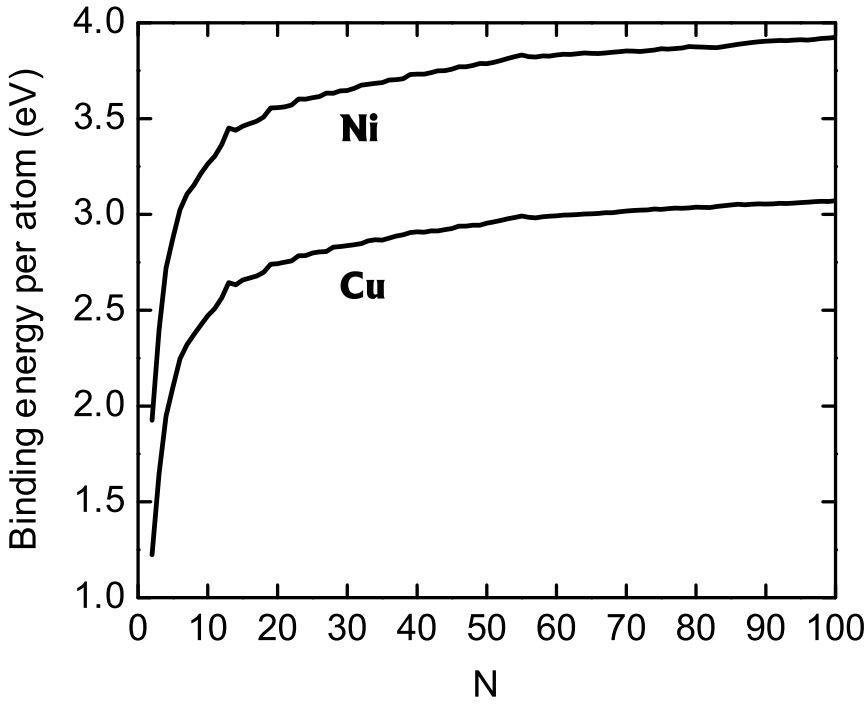

Figure 1: *Optimized binding energy per atom for Ni_N and Cu_N clusters with $2 \leq N \leq 100$.*

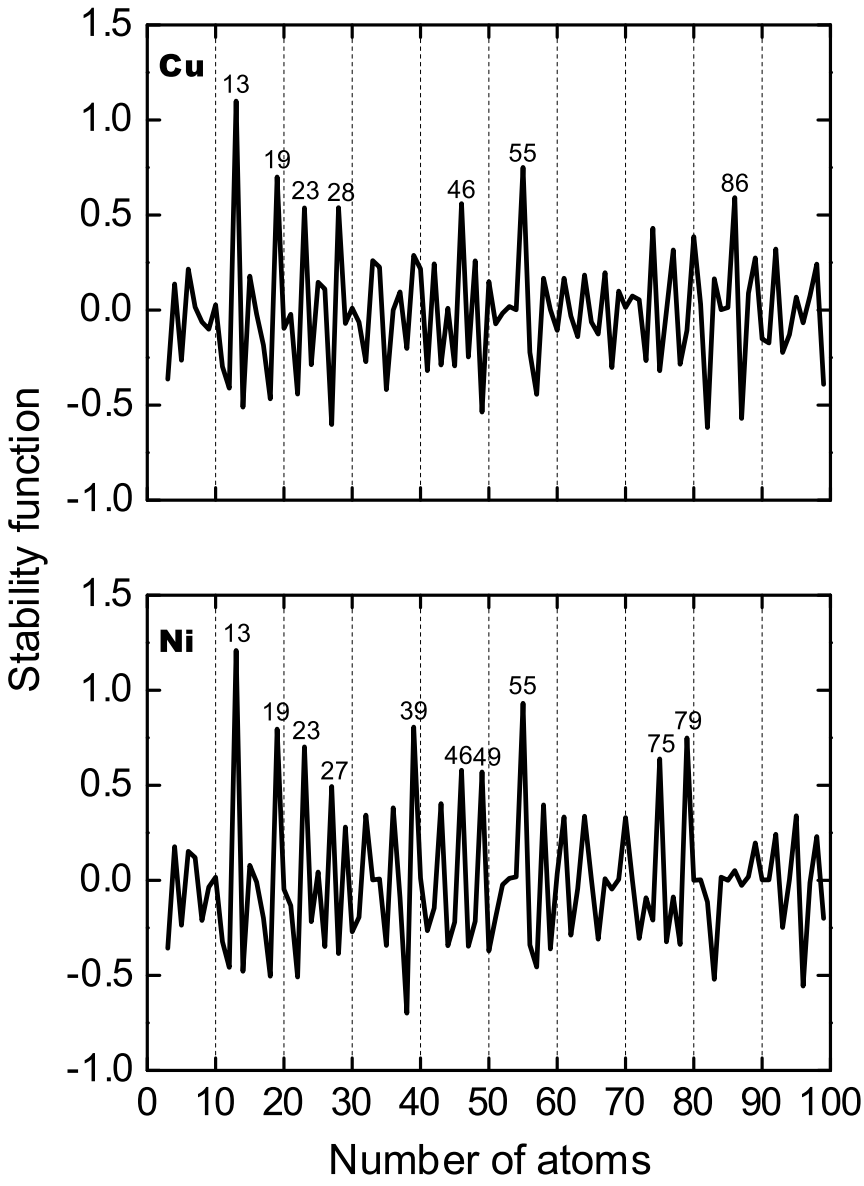

Figure 2: *The stability function for (lower panel) nickel and (upper panel) copper clusters with* $2 \leq N \leq 100$.

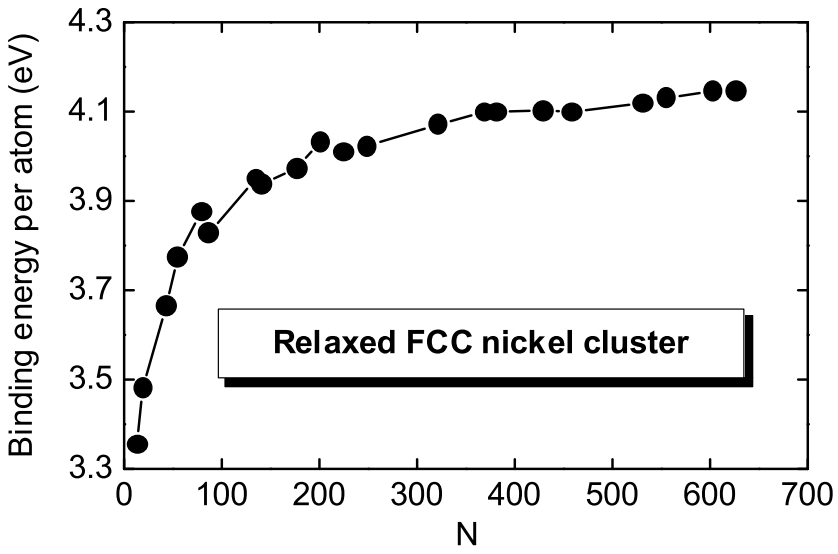

Figure 3: *The binding energy per atom for nickel clusters with* $2 \leq N < 700$. *Compared with Figure 1, here only relaxed finite segments of the FCC crystal structure were considered.*

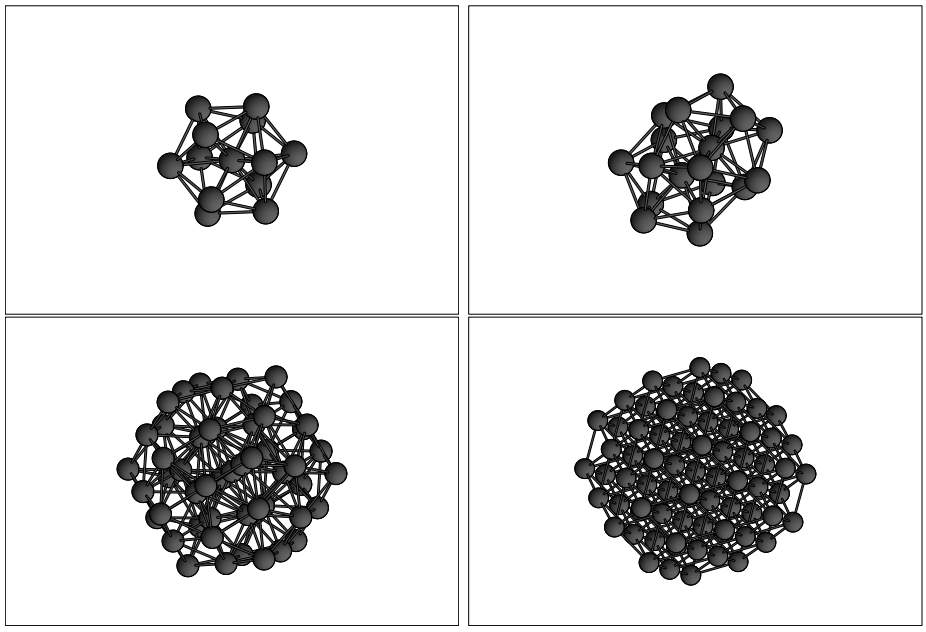

Figure 4: *Optimized structures of* Ni_{13}, Ni_{19}, Ni_{55} *and* Ni_{79}.

As an illustration of the application of our approach we show in Figure 1 the binding energy per atom for clusters of either nickel or copper atoms as a function of N up to $N = 100$. The results show that the binding energy per atoms roughly monotonically approaches the $N \to \infty$ value, although the curves have some structure that suggests the existence of magic numbers. In order to identify these clearly, the stability function

$$S(N) = E_{\rm tot}(N+1) + E_{\rm tot}(N-1) - 2E_{\rm tot}(N) \tag{8}$$

is particularly useful. This has maxima (minima) at particularly stable (unstable) structures and is shown in Figure 2 for the nickel and copper clusters. Comparing the two curves in Figure 2 shows that many magic numbers are similar for the two materials, but also that there are material-specific differences. It should be added at this point, that in [16] we compare our results with the somewhat limited information from more exact studies on smaller systems as well as with other theoretical and experimental information and found a very good agreement.

For $N \to \infty$ one would expect that the Ni clusters have the structure of the FCC crystal structure. We studied also finite segments of the FCC crystal structure obtained by considering spherical parts of the crystal structure with an atom at the center. Thereby, not all values of N can be considered, but, on the other hand, the structure optimization is orders of magnitude simpler thus allowing also systems with larger values of N to be considered. Figure 3 shows the resulting binding energy per atom. It turns out that for $N = 79$ the FCC structure is that of the lowest total energy of Figures 1 and 2. The structure of this system together with those of some smaller clusters are shown in Figure 4.

In contrast to the results obtained by considering only the spherical parts of the crystal structure, those of our '*aufbau/abbau*' approach permits a detailed study of a number of other properties:

1. The radial distribution of the atoms as a function of N. This gives information on whether the clusters grow in a shell-like fashion.

2. Starting with the optimized structures, a harmonic approximation can be used in calculating the vibrational properties.

3. These can in turn be used in calculating specific heat capacities as functions of N and temperature.

4. Through the knowledge of $E_{\rm tot}$ as a function of N for the complete series of N, dissociation channels can be identified.

5. The pair distribution function that is of experimental relevance and that gives information on structural characteristics.

6. The moments of inertia that give information of the overall shape of the clusters.

These studies are currently in progress and their results will be presented later.

4. SEMICONDUCTOR NANOPARTICLES

The existence of directional bonds for typical semiconductors implies that an accurate description of the properties of these materials has to include a treatment of the electronic orbitals. Also when using an efficient parameterized method like the one discussed in Sec. 2, the computational

costs are increased compared with those of the embedded-atom method. Accordingly, it becomes more difficult to carry through detailed structural studies. On the other hand, these directional, often tetragonal, bonds put also certain restrictions on the possible structures.

A further complication is that experimental studies on AB semiconductor nanoparticles often are carried through in some solution and that the nanoparticles often have surfactants that passivate dangling bonds. The fact that the precise size and stoichiometry of those often is not known does not make theoretical studies of their properties easier!

On the other hand, exactly the directional bonds suggest that the structure of the nanoparticles resembles that of the infinite crystal, at least in the inner parts of the nanoparticles. Therefore, as a first approximation one may study finite parts of the crystalline material. This approach is the one we have used in studying more different II-VI and III-V semiconductor nanoparticles and we shall here illustrate the approach by reviewing our results for CdS nanoparticles [17]. We would like to stress that despite these assumptions about the structure, our study represents one of the very few systematic studies of structure-property relations of such materials with more than roughly 50 atoms where structural degrees of freedom have been optimized.

An interesting property of the infinite CdS material is that the wurtzite and zincblende crystal structures are energetically very close [18] which may have interesting consequences for the finite systems. We studied accordingly finite parts of those two crystal structures obtained by considering spheres of different radii with the center at the mid-point of a Cd-S bond. Through this construction only stoichiometric Cd_nS_n nanoparticles are considered.

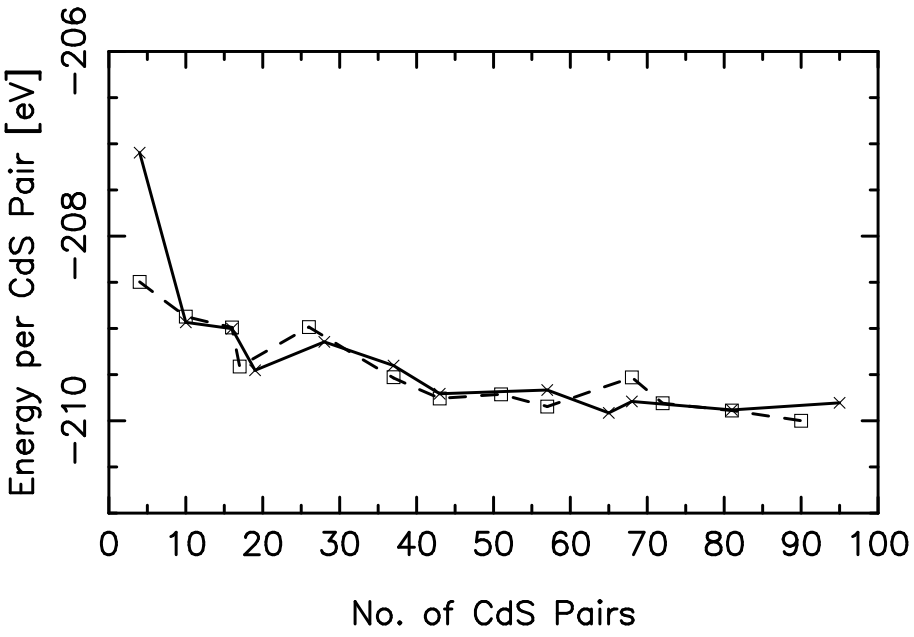

Figure 5: *Variation in the total energy per CdS pair as a function of n for zincblende- (solid curve) and wurtzite-derived Cd_nS_n clusters (dashed curve).*

It turned out (cf. Figure 5) that the relative stability for clusters derived from the two crystal structures in fact was dependent on the size of the system which actually also has been seen in experiment [19]. Further studies on other semiconductor nanoparticles (ZnO, CdSe, InP) have

given similar results.

For each structure the calculation leads to a large amount of information and in order to identify general trends we proceed as follows. First we define the center of the cluster

$$\vec{R}_0 = \frac{1}{N} \sum_{i=1}^{N} \vec{R}_i \tag{9}$$

where the summation runs over the N ($= 2n$ in our case) atoms. Subsequently

$$d_i = |\vec{R}_i - \vec{R}_0| \tag{10}$$

defines the distance of the ith atom to the center. We can then plot various properties as functions of d_i.

As one example, Figure 6 shows the number of atoms as a function of distance to the center both before and after structure relaxation. A Comparison of the two sets of curves for all the different clusters shows that — as expected — structural relaxations are confined to an outer region, whose thickness, moreover, is 2.5–3 Å independent of size and structure of the cluster. Furthermore, it turns out that in this surface region two types of relaxations occur: the metal (Cd) atoms move inward towards the center (the metal atoms seek a high coordination), whereas the sulphur atoms move outward (sulphur atoms are often satisfied with a lower coordination). These differences can not be identified in the curves in Figure 6.

The separation of the system into a bulk and a surface part can also be identified in the electronic properties. E.g., the radial distribution of the Mulliken populations of the valence electrons (cf. Figure 7) shows that in the inner parts these populations deviate only marginally from those of the neutral atoms (i.e., 12 for Cd and 6 for S), but in the surface region the atoms become significantly more ionic.

A further result was that the highest occupied molecular orbital (HOMO) is spread out over the entire cluster independent of n, whereas the lowest unoccupied molecular orbital (LUMO) is confined to the surface region. Therefore, the LUMO is very sensitive to the precise structure of the surface and its energy shows a much more irregular behaviour as a function of n compared to the energy of the HOMO. This also means that surfactants may modify first of all the energy of the LUMO. Excitons play an important role for these nanoparticles, and when assuming that the exciton wavefunction is derived first of all from those of the HOMO and LUMO, our results are in agreement with experimental findings that relaxation processes take place at low-symmetry sites, e.g., at the surface [20].

An interesting observation (Figure 8) is that there is a strong correlation between stability and band gap: large band gap implies larger stability. This can to some extent be considered a generalization of the results discussed above for the clusters of simple metals where the jellium model could be applied.

The overall behaviour of the band gap as well as of the total energy per atom pair is that they are decreasing as a function of nanoparticle size. The decrease of the band gap is observed experimentally: nanoparticles of different sizes have different colours, and the decrease of the total energy is similar to the results for the metal clusters. On the other hand, the fact that the total-energy curve is structured may imply that the size distribution for experimentally produced

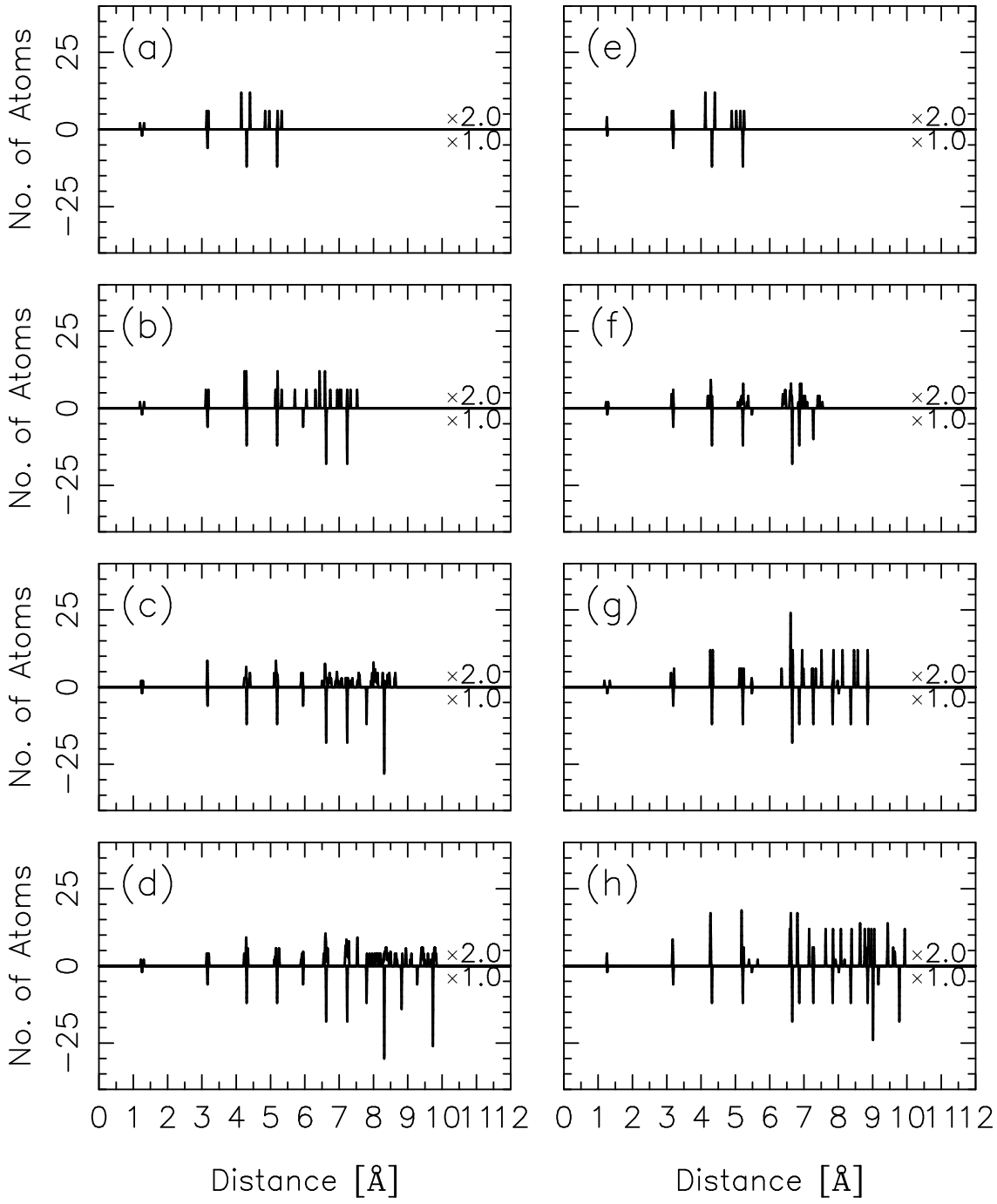

Figure 6: *Radial distribution of the atoms for zincblende- (left column) and wurtzite-derived CdS clusters (right column) with (a),(e) 16, (b),(f) 37, (c),(g) 57, and (d),(h) 81 atom pairs. The curves pointing upwards are for the optimized structures, whereas those pointing downwards are for the unrelaxed structures.*

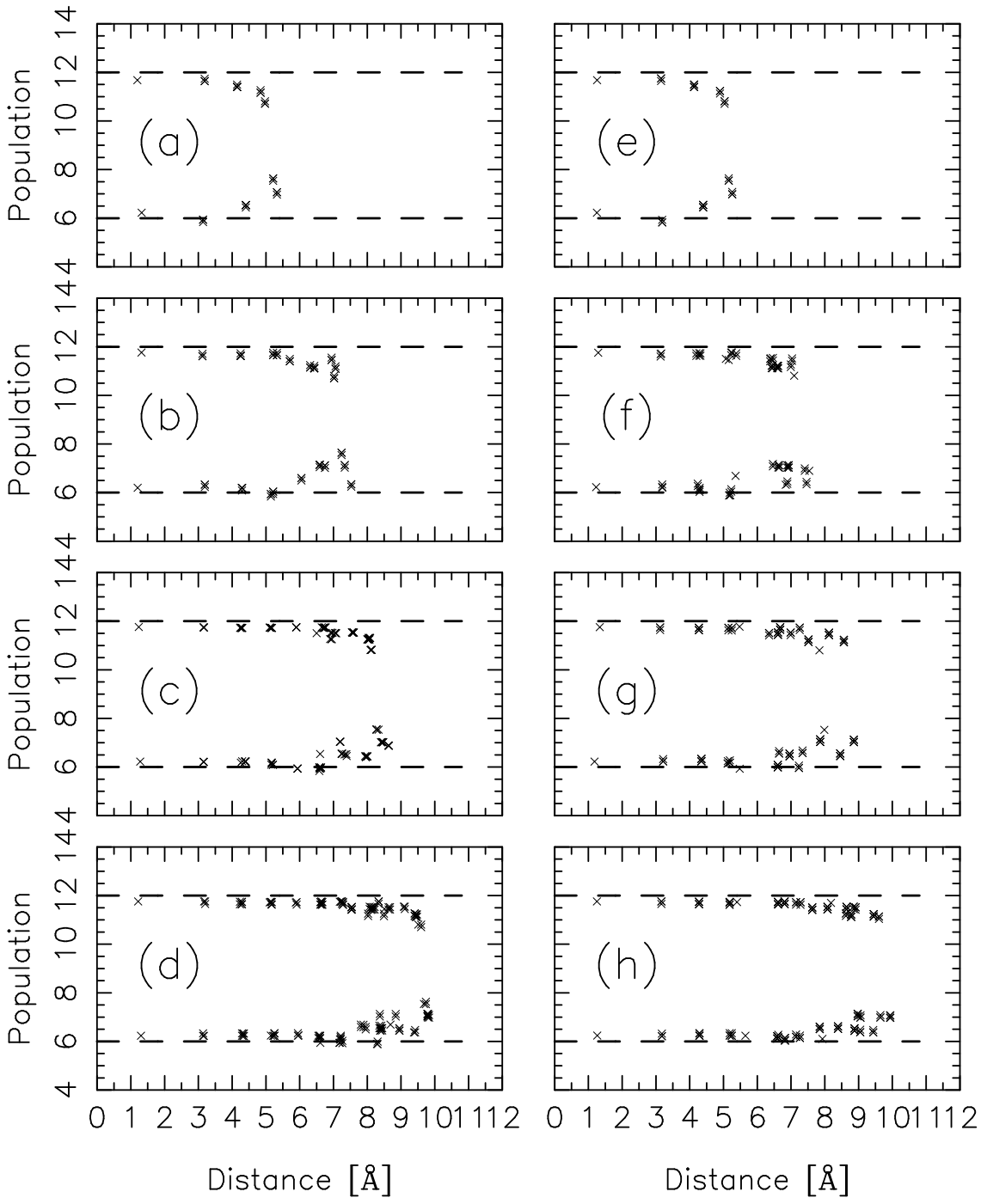

Figure 7: *Radial distribution of the Mulliken populations for zincblende- (left column) and wurtzite-derived CdS clusters (right column) with (a),(e) 16, (b),(f) 37, (c),(g) 57, and (d),(h) 81 atom pairs. The upper parts represent the values for the Cd atoms, and the lower ones those for the S atoms.*

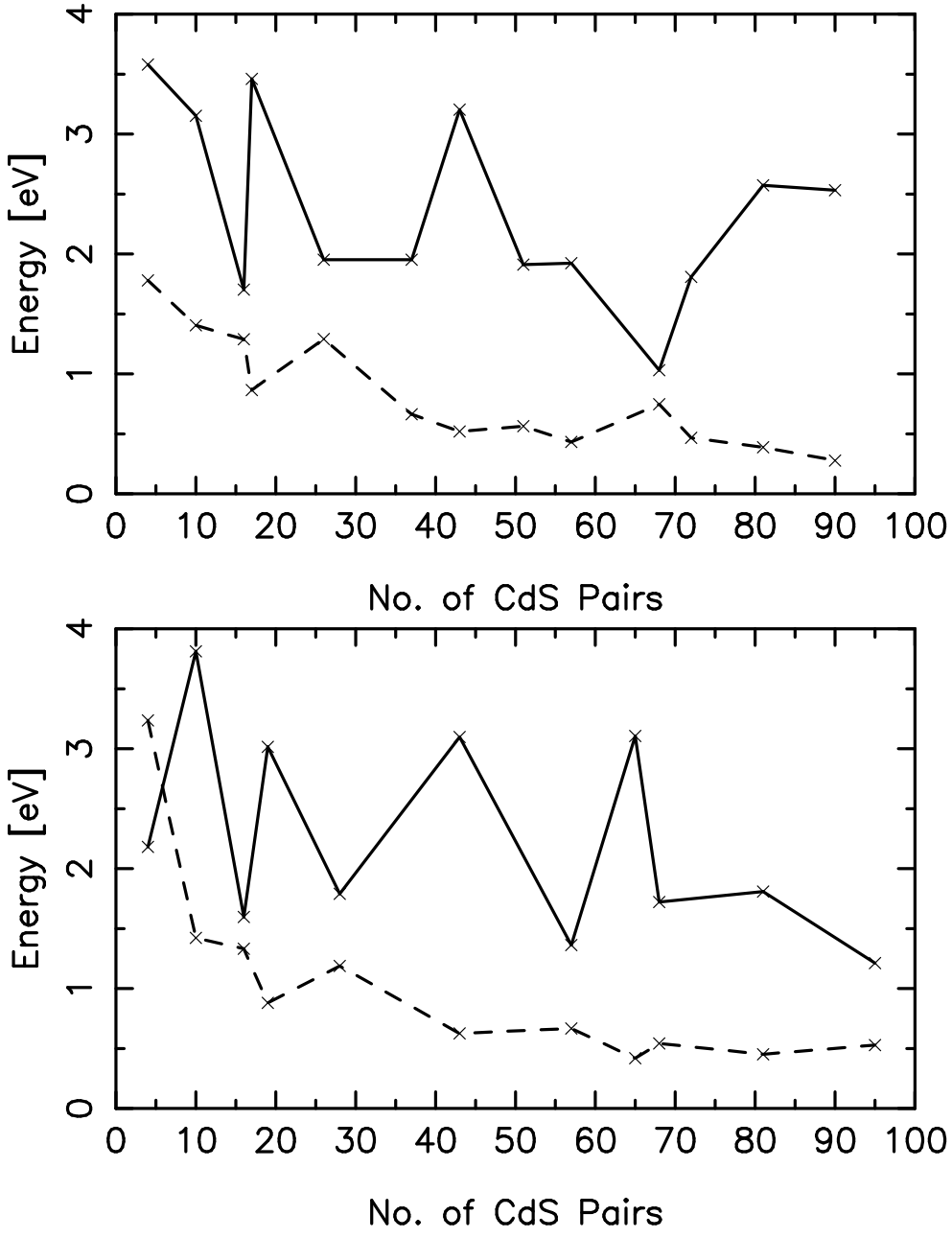

Figure 8: *HOMO-LUMO band gap (solid curve) and relative total energy per atom pair (dashed curve) for (lower part) zincblende- and (upper part) wurtzite-derived CdS clusters.*

samples is less regular than most often is assumed, which in turn could imply that only those clusters for which the stability (and hence band gap) is particularly large are produced. But once again, the presence of surfactants may modify this proposal.

5. METCARS

Let us now return to the materials that were discussed in the Introduction, i.e., the so-called metcars. Since these have directional bonds (for instance between the carbon atoms), the embedded-atom method is inapplicable and we have to use the computationally somewhat more heavy parameterized density-functional method. For a given Ti_mC_n cluster we know essentially nothing about the structure and in order to reduce the search for the global total-energy minimum in the $(3n+3m-6)$-dimensional space we have adapted the methods of genetic algorithms [21, 22]. The general idea behind these methods is that of combining the keeping of 'good building blocks' with randomness. This combination leads to a significant reduction in the number of structures for which the total energy shall be calculated but, nevertheless, we estimate that we in many cases need to consider 1–20 million structures.

There exist different variants of the genetic algorithms but let us describe one of those through a simple example. Let us assume we want to optimize the structure of a cluster of 20 identical atoms. We generate, e.g., 8 different structures at random. For each of those, separately, we find the closest local-total-energy minimum resulting in 8 — most likely different — structures. These 8 structures define the so-called parents. From these 8 we form 4 pairs at random. For any pair we cut each of the two clusters in two halves, whereby the directions of the normals to the cutting planes are generated randomly, and interchange one halfpart from each of the two clusters. Also for these so-called children (of which we have 8 in total) the closest local-total-energy minimum structures are calculated. Thereby we have in total 8 parents and 8 children and out of those 16 optimized structures we choose those 8 with the lowest total energy. These 8 define the parents of the next generation of clusters. This process is continued until the lowest total energy does not change any more as a function of generation number. It should be added that in practice one can never be sure that the last criterion is exactly fulfilled!

There are various ways of modifying this basic principle. E.g., instead of interchanging the halves of two clusters, one may consider only a single cluster for which the two pieces outside a random slice in the middle may be interchanged. Furthermore, so-called mutations may be introduced in which some randomly chosen atom may be moved at random with a certain probability.

We have generalized the method so that we can treat clusters with two types of atoms. Having established that the method worked (by studying Lennard-Jones clusters which are computationally easy to treat) we applied it to the metcars [23] and obtained the following results.

In Figure 9 we show the optimized structure of two of those metcars that turned out to have particularly high symmetry and that were aesthetically particularly appealing, i.e., the $(m,n) = (6,10)$ and $(m,n) = (8,12)$ metcars. Whereas the latter is the one that is well-known from experimental and theoretical studies (and in fact has a T_d symmetry as originally proposed by theory), to our knowledge the former plays essentially no role in experiment.

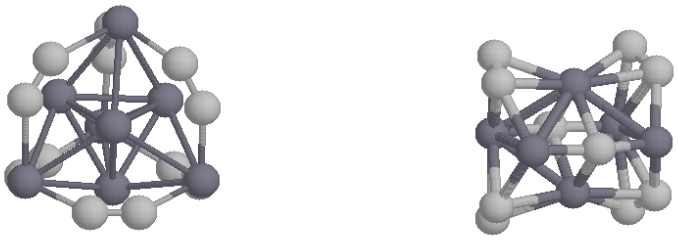

Figure 9: *Optimized structure of (right) Ti_6C_{10} and (left) Ti_8C_{12}. Light (dark) spheres represent C (Ti) atoms.*

The fact that the large abundance of the $(m, n) = (8, 12)$ metcar in experiment is obtained only under certain experimental conditions suggests that not only energetical arguments are required in explaining the special role of the $(m, n) = (8, 12)$ metcar. This is supported by the results presented in Figure 10. Here, we have considered the properties of the whole Ti_7C_n and Ti_8C_n series as functions of n. The energy gain upon addition of a C atom [i.e., $-E_{\rm tot}({\rm Ti}_m{\rm C}_n) + E_{\rm tot}({\rm Ti}_m{\rm C}_{n-1})$] shows that the $n = 12$ metcar is particularly stable for $m = 7$ but not for $m = 8$. Moreover, the correlation between stability and band gap that we observed for the semiconductor nanoparticles suggests that the $(m, n) = (8, 12)$ metcar is particularly unstable. And, finally, also in the number of nearest-neighbour bonds, the $(m, n) = (8, 12)$ metcar shows no particular properties. Thus, the somewhat disappointing conclusion of our study on the metcars is that total-energy arguments can not explain the experimentally observed large abundance of the $(m, n) = (8, 12)$ metcar but that, most likely, also kinetic effects play a significant role.

6. CONCLUSIONS

In this paper we have discussed the problems related to the determination of the structure of large but finite systems. We emphasized that it is important to identify clearly which properties are of interest in the theoretical studies and, accordingly, whether the structure of a local total-energy minimum, that of the global total-energy minimum, or just some realistic structure is required. Also in the computationally simplest case when 'just some realistic structure' is required, a systematic study of several different systems combined with the size and low symmetry of the individual systems make parameter-free first-principles calculations essentially too involved. Instead of limiting the number of structures and/or systems to very few as well as to impose certain, more or less justified, symmetry constraints we have chosen to use simpler computational methods like the embedded-atom method for metallic systems with delocalized electrons and a semi-empirical tight-binding method for systems with directional chemical bonds and localized electrons.

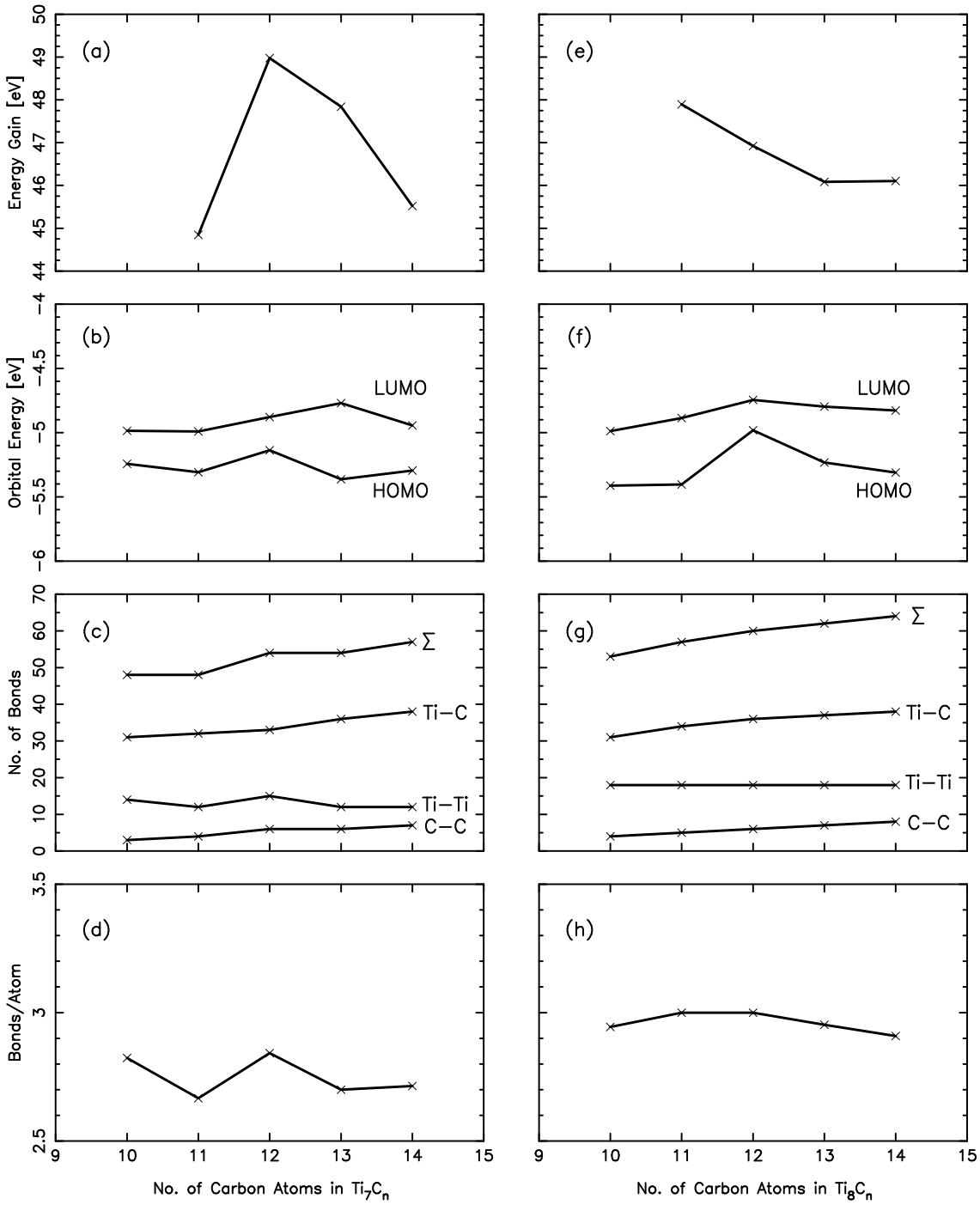

Figure 10: *(a),(e) Energy gain, (b),(f) HOMO and LUMO orbital energies, (c),(g) number of C–C, Ti–Ti, Ti–C bonds and their total number, and (d),(h) total number of bonds divided by total number of atoms for (left) Ti_7C_n and (right) Ti_8C_n as functions of n.*

With these choices we were able to study larger classes of systems systematically. For metallic clusters we presented a largely unbiased '*aufbau/abbau*' method (partly inspired by a simple picture about how clusters are formed in the gas phase) that allowed us to obtain very good candidates for the structures of the global total-energy minima for clusters with up to over 150 atoms. These results, obtained with the embedded-atom method, give immediately information about the so-called magic numbers and are currently been used in obtaining a number of other structural, vibrational, energetical, and thermodynamical properties.

The tight-binding method is computationally somewhat heavier than the embedded-atom method and a systematic study like the one for the metal clusters was only possible if further restrictions were made on the structure. We considered, as one example, stoichiometric CdS nanoparticles derived from either the zincblende or the wurtzite crystal structure. Our results, that we have seen confirmed for other stoichiometric and non-stoichiometric semiconductor nanoparticles, showed a clear size-dependence of the relative stability of the two types of structures. Moreover, we observed a well-defined separation into a bulk and a surface part. Most interesting was a correlation between HOMO/LUMO energy gap and stability as well as the fact that neither of these two quantities was a monotonic function of the size of the system. These results may have important consequences for the size distribution of the experimentally produced nanoparticles.

Finally, the Ti_mC_n metcars represented a class of materials where an essentially unbiased structure optimization was important. To this end we used a variant of the so-called genetic algorithms which was described in some detail. To our surprise the results for the metcars were not able to explain the large abundance of the Ti_8C_{12} metcar that is observed in *some* experiments (depending on the experimental conditions). This we interpret as meaning that this experimental result is determined largely by kinetic effects.

ACKNOWLEDGMENTS

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