HCM Newsletter

Ψ_k Network

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

Number 12 December 1995

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Editorial

The **Editorial** is followed by the section **News from the Network**. In this section readers can find information by Volker Heine (the chairman of the Network Management Board) on *Collaborative and Training Projects* established at the recent meeting of the *Network Management Board.* Moreover, there we also write about the need of receiving all possible information from those of you who in any way benefited from the Network in your research.

In the section **News from the Working Groups** readers will find reports on recent collaborative visits and workshops. These are followed by job announcements.

The **Abstracts Section** is followed by the section **Presenting Other HCM Projects** where we have an article by *Chris Ewels* (Exeter) on his research done in CINECA (Bologna) using the High Performance Computing Facility within the HCM Programme *ICARUS Scheme.* In this article readers can also find information on how to apply and make use of this and other similar facilities supported by the HCM Programme.

In the **Highlight of the Month** section we have an article by *Peter Zahn, I. Mertig, Manuel Richter and Helmut Eschrig* on *"Ab-initio Calculation of Giant Magnetoresistance in Magnetic Multilayers".*

Finally, partly due to their complicated nature, the **Announcement of the Bond Order Potentials Workshop**, the **Announcement of the OXYGEN 1996 Workshop**, and the **2nd Circular of the Network Conference** are placed at the very end of the *Newsletter.* The **2nd Circular** refers to a conference suggestion form *form.tex* which calls upon a formatting file *psik.sty.* The LaTeX file of the suggestion form, *form.tex*, as well as the *psik.sty* file, are attached at the end of the LaTeX file of this *Newsletter*, just after the "`\end{document}`". In order to create a printed version of the suggestion form one needs to save all these files separately, and process `form.tex` independently from `newsletter_12.tex` file, containing the main body of the *Newsletter.* Please note that those of you who normally receive only the postscript file of the *Newsletter* will additionally receive the conference suggestion form as a separate postscript file: `form.ps`.

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

http://www.dl.ac.uk/TCSC/HCM/PSIK/main.html

This also contains pointers to several other nodes: *O.K. Andersen (Stuttgart)* which includes information on the **Network Conference**, *M. Gillan (Keele)*, *B.L. Gyorffy (Bristol)*, *J. Nørskov (Lyngby)* with information on CAMP, *M. Scheffler (FHI Berlin)*, and *A. Walker (UEA Norwich)*. If you maintain a home page on your activities we will be happy to include a pointer from the *Network's* home page to your home page.

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

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

	function
psik-coord@daresbury.ac.uk	**messages to the coordinator & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB**
psik-network@daresbury.ac.uk	**messages to the whole Network**

Dzidka Szotek & Walter Temmerman
e-mail: psik-coord@daresbury.ac.uk

News from the Network

Money, *Money*, Money, ..., *MONEY*

That has caught your attention: good!

The Network has money and would like to see more collaborations. The main requirement is that first class science results, with publications. The main boundary conditions are that we can only pay subsistance (now up to 60 ECU per day) plus travel, not salary or equipment. Also, both collaborators must be from an organisation that is a node of the Network.

The Network is offering 10 grants for Collaboration and Training Projects of 2000 ECU each. Together with the availability of email that should be enough to get a collaboration going. Once it is up and running, further applications can be made in the normal way.

There are many different types of collaboration. Perhaps an ideal one would involve a younger scientist learning a new code to establish a new line of research at his/her home university: but we are flexible.

Two words of advice to those wishing to start a collaboration. Firstly, what benefit does the other partner get from the collaboration? Perhaps you can help further his/her research intrests with modest input in time and effort on his/her side. Secondly, remember codes are shared in the Network through genuine collaborations with the originator sharing control of the project and the way his/her code is used, plus having his/her name on the research papers.

The procedure is to approach the person or group you want to collaborate with, formulate the project and submit it as a Collaborative and Training Project with a budget to the appropriate Working Group Spokesperson (details of the names and addresses can be found in the Network's Newsletter No. 1) or to myself as Network's Chairman, or to Ole K. Andersen (oka@radix2.mpi-stuttgart.mpg.de) as Vice-Chairman, or to Walter M. Temmerman (w.m.temmerman@dl.ac.uk) as the Network's Coordinator.

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What impact has the Network had on your research?

Since the Network is coming up for renewal next year, we would like to appeal to those of you who in any way benefited from the Network in your research to write to us about it. It appears that all the workshops, ”hands-on a computer code” and others, organised by the Network during the last year and a half, emerge as the Network's key deliverable and will impact on the renewal of the Network and future of science in different universities and countries.

Therefore, if you have participated in any of the workshops organised by the Network we would appreciate if you could contact us and provide an information what impact has the workshop or an acquired code had on your research. Have you used the code or the knowledge that you have gained at the workshop for your research? Have you published any papers whose results benefited from the code or workshop in general, and most importantly, have you acknowledged the code and the Network, as the organiser of the workshop, in any of your papers? We would also be interested in establishing the multiplication effect: we started it.

This information is of paramount importance for monitoring the impact that our HCM Network has had on research of people in general, and in particular, of those who in any way have benefited from the Network. Moreover, this information we need to submit to Brussels in the form of an annual report on Network's activity, but is also going to be used to support our application for the renewal of the Network. We are not able to contact each of you individually, in many cases we do not have your present e-mail addresses etc. So, please do get back to us if you have anything to tell us on the above matters. Even if you do not use the code that you have acquired or knowledge that you have gained at any of the workshops; perhaps because you have found out why it cannot be of use to you, we would also like to hear it.

We do also desperately need all information on publications that acknowledge the *Network* explicitly, and which resulted from collaborations or other activities within the Network.

If any of you published or submitted for publication such papers where the *Network* had been acknowledged, we would like to hear from you. Could you please just send us detailed references of such papers, namely the authors, journal (volume, page, year) and the title of the paper. We would not like to miss any of such publications.

News from the Working Groups

Report on the collaborative visit of C.M.J. Wijers (Twente) to N. Christensen (Aarhus)

2 November, 1995

The issues of the visit were twofold: 1) to discuss a common project to be performed by a graduate student, Mr. Ivo Wenneker, from Twente University 2) to give a lecture about the present status of the Twente discrete cellular project. The abstract of this lecture follows here below.

Discrete Cellular Methods: Maxwell's comeback?

C.M.J. WIJERS,
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Large inhomogeneous systems like large molecules or surfaces, display optical responses deviating from the results of standard theoretical treatments. Those deviations can be amplified by using difference, anisotropic difference, SHG or optical scattering experiments. Electrodynamics offers two alternatives for the description of such phenomena: continuum or discrete, and both approaches have a sizeable record in physics. For solid state optics only the continuum description has been used to link the electrodynamics to the underlying quantum mechanics of the system. In this lecture arguments will be collected that it makes sense to look for the quantum mechanical roots of discrete models. If such link can be achieved, one gains immediately the ability of discrete models to handle directly a lot of different geometries. This pays off directly for large inhomogeneous systems. It turns out however that the link to quantum mechanics for discrete models is not a simple analogy of the continuum case. A necessary consequence of electrodynamic discreteness, is the introduction of cells in quantum mechanics. This means that we have to study open quantum mechanical systems. Another consequence is also that besides electrodynamical nonlocal interactions also quantum mechanical nonlocality needs to be taken into account. The talk will give (and trigger?) further discussion how to make discrete cellular methods work.

As to the first item: Both groups are working on a full potential version of their electronic structure packages. The techniques used in the two groups, the LMTO-types and the CLOPW-types, have distinct advantages for different applications. In calculating NMR-spectra for heavy metals, a CLOPW-type of calculation might be supportive for the LMTO-type of calculation. This comparative study between the two methods, will be the research topic for the graduate student in his 4 month stay at Aarhus.

(C.M.J. Wijers)

Report on the collaborative visit of Pietro Ballone ((MPI-FKF, Stuttgart) to Cambridge

21-25 October, 1995

Discussions were held with the group of Mike Payne and Volker Heine in the Cavendish Laboratory on Monday 23 October on technical aspects of total energy calculations with pseudopotentials and plane waves, and their applications. Tuesday 24 October was taken up with a Minerals Physics Workshop in Cambridge, at which a report was given on the calculation of phase transitions under pressure of magnesium silicate. Arrival on Saterday to get air fare reduction. Only part of the cost is claimed from the Network, namely 70 pounds for accomodation in Cambridge. Charge: Cambridge node, pseudopotential working group.

(V. Heine)

Report on
Fourth Central European Workshop on Electronic and Magnetic Properties of Alloys, Surfaces and Interfaces
2–5 October, 1995

This workshop was organized by the Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, and the Institute of Physics, Academy of Sciences of the Czech Republic, Prague, and was financially supported by the Brno Trade Fairs and Exhibitions Co. Ltd., Czechoslovak Trade Bank and Czech Saving Bank. It was a follow up of the preceding meetings: in Vienna (P. Weinberger, 1992), in Budapest (J. Kollár, 1993), and in the Swiss mountain village Stels (R. Monnier, 1994).

The 1995 workshop took place in the Holiday Center of the Brno Trade Fairs and Exhibitions in Zubří, Czech Republic, in the heart of the Czech-Moravian Highlands. It was attended by 34 scientists from 10 different countries, all of whom were practicioners of Green's function techniques and full-potential methods for electronic structure calculations in alloys, surfaces and interfaces. There were many interesting talks and plenty of opportunities for participants to discuss their recent work. The scientific program follows below.

The next, fifth, workshop is planned for the autumn of next year in Vienna.

(Mojmír Šob, Ilja Turek, Josef Kudrnovský, Václav Drchal)

Scientific Program

Magnetic coupling and anisotropy

P. H. Dederichs
Interlayer coupling and quantum well states in Co/Cu layers

L. Szunyogh, P. Weinberger and B. Újfalussy
Fully relativistic spin-polarized study of Fe multilayers in Au(001)

B. Újfalussy, L. Szunyogh and P. Weinberger
Studies of magnetic anisotropy in Fe-Cu over- and interlayers

Magnetic coupling and GMR

J. Mathon
Quantum well theory of the exchange coupling in magnetic multilayers

J. Kudrnovský, V. Drchal, I. Turek, M. Šob and P. Weinberger
Interlayer magnetic coupling: effect of disorder in spacer

I. Mertig, P. Zahn, M. Richter and H. Eschrig
Ab-initio calculations of giant magnetoresistence

Alloys

A. V. Ruban and **H. L. Skriver**
Calculated site substitution in γ'-Ni$_3$Al

V. Drchal, J. Kudrnovský, I. Turek and A. Pasturel
Ab-initio theory of surface segregation in random alloys

T. Schulthess and **R. Monnier**
Influence of charge correlations on the surface energy, work function and surface composition of random binary alloys

P. Weinberger
Electrical conductivity in semi-infinite systems

A. B. Shick, V. Drchal and J. Kudrnovský
Relativistic spin-polarized TB-LMTO method: application to magnetic properties of random alloys and their surfaces

H. Ebert and G.-Y. Guo
Theoretical investigation of the magnetic X-ray dichroism in diluted and concentrated transition metal alloys

J. Banhart and H. Ebert
Ab-initio theory of spontaneous galvanomagnetic effects in random alloys

Full-potential methods

L. Vitos, **J. Kollár** and H. L. Skriver
Full charge density scheme: application for shear deformations

O. Genser, A. Biedermann, **J. Redinger** and P. Varga
Surface electronic structure of p-d bonded systems: Some recent results

C. Blaas
High resolution Compton scattering in Fermi surface studies

R. Stadler, W. Wolf, G. Kresse, J. Furthmüller, **R. Podloucky**
and J. Hafner

Electronic structure, elastic constants and phonon dispersion of $CoSi_2$

F. Máca and M. Scheffler
Electronic structure and STM image of a p(2x2) composite double layer ordered surface alloy of Na on Al(111)

L. Steinbeck, M. Richter, U. Nitzsche and **H. Eschrig**
Ab-initio calculation of electronic structure, crystal field, and intrinsic magnetic properties of Sm_2Fe_{17}, $Sm_2Fe_{17}N_3$, $Sm_2Fe_{17}C_3$ and Sm_2Co_{17}

New methods

P. Miller and **B. Gyorffy**
On the mechanism of the de Haas–van Alphen oscillations in
the superconducting state

I. Turek, J. Kudrnovský, M. Šob and V. Drchal
Surface magnetism of random binary transition-metal alloys

L. Udvardi, L Szunyogh and R. Király
Magnetic anisotropy on overlayers

B. Velický, H. Eschrig, K. Koepernik, A. Ernst and R. Hayn
Towards ab-initio CPA for alloys using mixed basis set

C. Barreteau and **F. Ducastelle**
Quantitative transmission electron microscopy in disordered alloys

J. Vackář, **A. Šimůnek** and R. Podloucky
Ab-initio pseudopotentials of interacting atoms

Announcement

Ph. D. Position

University of Sheffield (UK)

A Ph. D. studentship is available as soon as possible to work with Professor Gillian Gehring (University of Sheffield) and Dr. Walter Temmerman (Daresbury Laboratory) on the total energy and Fermi surface studies of the heavy fermion compounds.

A prospective student will be expected to make a detailed study of UBe_{13}. This is expected to help the interpretation of the planned de Haas van Alphen experiments in Professor Mike Springford's group (University of Bristol). The theoretical study will involve both development or generalisation of computer codes and necessary calculations.

To apply, please send your CV and letter of application to the addresses below either by normal or electronic (only postscript or LaTeX files are acceptable) mail.
Further information can be obtained from:

Dr. W.M. Temmerman,
Daresbury Laboratory,
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Announcement

Postdoctoral Research Positions in Electronic Structure Theory of Solids

Solid State Theory Group
Basic Sciences Division
National Renewable Energy Laboratory
Golden, Colorado 80401, USA

The Solid State Theory Group at the National Renewable Energy Laboratory invites applications for two postdoctoral research positions, one beginning January, 1996, and one beginning September, 1996. The positions are for two years, renewable upon mutual agreement to a third year. The Solid State Theory Group currently consists of eight Ph.D.'s in condensed matter theory and interacts with a broad range of experimentalists in semiconductor physics at NREL. Areas of particular interest include first-principles electronic structure theory of semiconductor nanostructures and superlattices and the theory of phase-stability of metallic alloys. Candidates should send a curriculum vitae, list of publications (including preprints of unpublished papers, if possible) and list of three references to:

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

NREL is an equal opportunity/affirmative action employer. Clarifications or further details can be obtained via e-mail to **alex_zunger@nrel.gov**.

Noncollinear Magnetic Order and Electronic Properties of U_2Pd_2Sn and U_3P_4

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Abstract

We report results of calculations that explain in the itinerant electron picture the noncollinear magnetic structure observed in the two very different compounds U_2Pd_2Sn and U_3P_4. We use the local approximation to spin-density functional theory and the ASW method incorporating spin-orbit coupling (SOC), noncollinear moment arrangements and an effective orbital field responsible for Hund's second rule. We show how the relativistic effect of SOC and the particular symmetry properties of the compounds cooperate and lead to noncollinear magnetic structures, in the case of U_2Pd_2Sn to an antiferromagnetic and in the case of U_3P_4 to a ferromagnetic structure the latter possessing a weak antiferromagnetic component.

(submitted to Physica B)
Revtex version can be obtained from: dg5m@mad1.fkp.physik.th-darmstadt.de
(L. Sandratskii)

This work has benefited from collaborations within the EU Human Capital and Mobility Network on *"Ab initio (from electronic structure) calculation of complex processes in materials"* (contract:
ERBCHRXCT930369).

Ab initio pseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach

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Abstract

The ground-state properties of Fe, Co, and Ni are studied with the linear-augmented-plane-wave (LAPW) method and norm-conserving pseudopotentials. The calculated lattice constant, bulk modulus, and magnetic moment with both the local-spin-density approximation (LSDA) and the generalized gradient approximation (GGA) are in good agreement with those of all-electron calculations, respectively. The GGA results show a substantial improvement over the LSDA results, i.e., better agreement with experiment. The accurate treatment of the nonlinear core-valence exchange and correlation interaction is found to be essential for the determination of the magnetic properties of $3d$ transition metals. The present study demonstrates the successful application of the LAPW pseudopotential approach to the calculation of ground-state properties of magnetic $3d$ transition metals.

(Submitted to Phys. Rev. B)
REVTEX version can be obtained from: `cho@theo21.RZ-Berlin.MPG.DE`

Six-Dimensional Quantum Dynamics of Adsorption and Desorption of H_2 at Pd(100): Steering and Steric Effects

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Abstract

We report the first six-dimensional quantum dynamical calculations of dissociative adsorption and associative desorption. Using a potential energy surface obtained by density functional theory calculations, we show that the increase of the sticking probability with decreasing kinetic energy at low kinetic energies in the system H_2/Pd(100), which is usually attributed to the existence of a molecular adsorption state, is due to dynamical steering. In addition, we examine the influence of rotational motion and orientation of the hydrogen molecule on adsorption and desorption.

(Submitted to Phys. Rev. Lett.)
REVTEX version can be obtained from: `axel@theo22.RZ-Berlin.MPG.DE`

Enhanced electron-phonon coupling at the Mo and W (110) surfaces induced by adsorbed hydrogen

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Erio Tosatti
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International School for Advanced Studies (SISSA)
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Abstract

The possible occurrence of either a charge-density-wave or a Kohn anomaly is governed by the presence of Fermi-surface nesting and the subtle interaction of electrons and phonons. Recent experimental and theoretical investigations suggest such an effect for the hydrogen covered Mo and W (110) surfaces. Using density-functional theory we examine the electronic structure and the electron-phonon coupling of these systems. Besides good agreement with the experimental phonon frequencies our study provides a characterization and quantitative analysis of an unusual scenario determining the electronic, vibrational, and structural properties of these surfaces.

(Submitted to Phys. Rev. Lett.)
REVTEX version can be obtained from: `kohler@theo26.RZ-Berlin.MPG.DE`

Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code `WIEN`

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Robert Kouba and Claudia Ambrosch-Draxl
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Abstract

Following the approach of Yu, Singh, and Krakauer [Phys. Rev. B **43** (1991) 6411] we extended the linearized augmented plane wave code `WIEN` of Blaha, Schwarz, and coworkers by the evaluation of forces. In this paper we describe the approach, demonstrate the high accuracy of the force calculation, and use them for an efficient geometry optimization of poly-atomic systems.

(Submitted to Comp. Phys. Commun.)
Postscript version can be obtained from: `kohler@theo26.RZ-Berlin.MPG.DE`

This work has benefited from collaborations within the EU Human Capital and Mobility Network on *"Ab initio (from electronic structure) calculation of complex processes in materials"* (contract:
ERBCHRXCT930369).

Theoretical study of O adlayers on Ru (0001)

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Abstract

Recent experiments performed at high pressures indicate that ruthenium can support unusually high concentrations of oxygen at the surface. To investigate the structure and stability of high coverage oxygen structures, we performed density functional theory calculations, within the generalized gradient approximation, for O adlayers on Ru (0001) from low coverage up to a full monolayer. We achieve quantitative agreement with previous low energy electron diffraction intensity analyses for the (2×2) and (2×1) phases and predict that an O adlayer with a (1×1) periodicity and coverage Θ=1 can form on Ru (0001), where the O adatoms occupy hcp-hollow sites.

(Submitted to Phys. Rev. B)
REVTEX version can be obtained from: `cts@theo21.RZ-Berlin.MPG.DE`

Potential Energy Surface for H_2 Dissociation over Pd(100)

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Abstract

The potential energy surface (PES) of dissociative adsorption of H_2 on Pd(100) is investigated using density functional theory and the full-potential linear augmented plane wave (FP-LAPW) method. Several dissociation pathways are identified which have a vanishing energy barrier. A pronounced dependence of the potential energy on "cartwheel" rotations of the molecular axis is found. The calculated PES shows no indication of the presence of a precursor state in front of the surface. Both results indicate that steering effects determine the observed decrease of the sticking coefficient at low energies of the H_2 molecules. We show that the topology of the PES is related to the dependence of the covalent H(s)-Pd(d) interactions on the orientation of the H_2 molecule.

(Submitted to Phys. Rev. B)
REVTEX version can be obtained from: `swilke@vnatolisgi.erenj.com`

Scattering of rare-gas atoms at a metal surface: evidence of anticorrugation of the helium-atom potential-energy surface and the surface electron density

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Abstract

Recent measurements of the scattering of He and Ne atoms at Rh (110) suggest that these two rare-gas atoms measure a *qualitatively* different surface corrugation: While Ne atom scattering seemingly reflects the electron-density undulation of the substrate surface, the scattering potential of He atoms appears to be anticorrugated. An understanding of this perplexing result is lacking. In this paper we present density functional theory calculations of the interaction potentials of He and Ne with Rh (110). We find that, and explain why, the nature of the interaction of the two probe particles is qualitatively different, which implies that the topographies of their scattering potentials are indeed anticorrugated.

(Submitted to Phys. Rev. Lett.)
REVTEX version can be obtained from: `paolo@theo24.RZ-Berlin.MPG.DE`

Unusually Large Thermal Expansion of Ag(111)

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Abstract

We investigate the thermal behavior of the (111) surface of silver, using phonon frequencies obtained from *ab initio* total energy calculations, and anharmonic effects treated within a quasiharmonic approximation. Our results reproduce the experimental observation of a large and anomalous increase in the surface thermal expansion at high temperatures [P. Statiris *et al.*, Phys. Rev. Lett. **72**, 3574 (1994)]. Surprisingly, we find that this increase can be attributed to a rapid softening of the *in-plane* phonon frequencies, rather than due to the anharmonicity of the out-of-plane surface phonon modes. This provides evidence for a new mechanism for the enhancement of surface anharmonicity. A comparison with Al(111) shows that the two surfaces behave quite differently, with no evidence for such anomalous behavior on Al(111).

(Submitted to Phys. Rev. Lett.)
REVTEX version can be obtained from: `shobhana@theo26.RZ-Berlin.MPG.DE`

Electronic Structure of $PrBa_2Cu_3O_7$: A local-spin-density approximation with on-site Coulomb interaction calculation

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Abstract

Electronic structure calculations based on the local-spin-density approximation fail to reproduce the antiferromagnetic ground state of $PrBa_2Cu_3O_7$ (PBCO). We have performed LMTO-ASA calculations, based on the local-spin-density approximation with on-site Coulomb correlation applied to Cu(1) and Cu(2) $3d$ states. We have found that inclusion of the on-site Coulomb interaction modifies qualitatively the electronic structure of PBCO with respect to the LSDA results, and gives Cu spin moments in good agreement with the experimental values. The Cu(2) upper Hubbard band lies about 1 eV above the Fermi energy, indicating a Cu^{II} oxidation state. On the other hand, the Cu(1) upper Hubbard band is located across the Fermi level, which implies an intermediate oxidation state for the Cu(1) ion, between Cu^{I} and Cu^{II}. The metallic character of the CuO chains is preserved, in agreement with optical reflectivity [K. Takenaka *et al.* Phys. Rev. B **46**, 5833 (1992)] and positron annihilation experiments [L. Hoffmann *et al.* Phys. Rev. Lett. **71**, 4047 (1993)]. These results support the view of an extrinsic origin of the insulating character of $PrBa_2Cu_3O_7$.

(Submitted to Phys. Rev. B)

Manuscripts available from: biagini@imoax1.unimo.it

High Resolution Compton Scattering in Fermi Surface Studies: Application to FeAl

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Abstract

We present a novel theoretical approach to identify Fermi surface contributions in high resolution Compton scattering data. For FeAl Compton profiles we show that the Fermi-surface-related features (occupation of states) can be separated from those originating from the spatial extent of the wave functions. The first high resolution Compton scattering experiment done at the European Synchrotron Radiation Facility confirms these findings. This technique opens up new possibilities especially in Fermiology studies of high temperature superconductors.

(Phys. Rev. Lett. **75**, 1984 (1995))
Reprints available from: cb@eecws6.tuwien.ac.at

Fully relativistic spin–polarized description of interface exchange coupling: Fe multilayers in Au(100)

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Abstract

The spin-polarized fully relativistic Screened Korringa-Kohn-Rostocker method is applied to calculate magnetic anisotropy energies for Fe multilayers in Au(100), separated by up to 16 spacer layers of Au. With respect to the antiparallel as well as to a perpendicular relative orientation of the magnetization in the Fe slabs these anisotropy energies as calculated (a) in terms of total energies, (b) within the force theorem approximation and (c) within the frozen potential approximation are discussed using the concept of layer-resolved quantities. In particular the comparison between the total energy and the force theorem approach is presented in some detail because of possible implications for an ab-initio description of transport properties in multilayer systems.

(submitted to Phys. Rev. B)
Manuscripts available from: pw@eecws1.tuwien.ac.at

Acid-base catalysis in zeolites from first principles

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Abstract

Zeolite materials are microporous aluminosilicates with various uses, including acting as important catalysts in many processes. One such process is the methanol to gasoline reaction, used widely in industry. This reaction is known to be associated with Brønsted acid sites in the zeolite, formed when Si is substituted by Al in the framework, with an associated H^+ being bound nearby to maintain charge neutrality. However it is not clear exactly what role the proton plays in this reaction.

Because of the large unit cell (generally 50-300 atoms, depending on the particular zeolite) of such structures, most ab initio calculations of these materials have focussed on studying small clusters representing just a portion of the framework. However, by choosing the chabazite zeolite structure, which has only 36 atoms in the primitive unit cell, we have been able to perform a full periodic ab initio calculation. This has used density functional theory with a generalised gradient approximation for the exchange-correlation energy, a plane-wave basis set, and norm-conserving optimised pseudopotentials. Using these methods we have examined the geometry and electronic structure of a zeolite acid site, and considered one way in which a methanol molecule may bind to such a site.

(Intl. J. Quant. Chem., in press)

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The mechanism of tritium diffusion in lithium oxide

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Abstract

Lithium oxide is a possible candidate for a breeder blanket material in fusion reactors. Tritium is generated in the material, which can be extracted and fed into the fusion reactor to help sustain the fusion reaction. Experimental studies have shown the extraction rate is controlled by diffusion of tritium in the bulk, but the exact mechanism is not clear.

Here we present ab initio density functional calculations of the various diffusion pathways which have been suggested, including the diffusion of tritium as an interstitial and various vacancy assisted mechanisms. The activation energy has been calculated for each pathway, and by comparison with experimental results we have deduced which mechanism is most likely. This is shown to be a simple two-stage swapping of a lithium and tritium ion.

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Time-dependent density functional theory beyond linear response: an exchange-correlation potential with memory

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Abstract

We propose a memory form of exchange-correlation (xc) potential $v_{xc}(\mathbf{r}, t)$ for time-dependent interacting many-particle systems. Unlike previous memory-xc potentials, our v_{xc} is not limited to the linear response regime. The proposed form of v_{xc} has the maximum degree of spatial locality allowable in view of constraints imposed by Galilean invariance and by the Harmonic Potential Theorem. For the case of the inhomogeneous electron gas, we give an explicit prescription for v_{xc} based solely on an existing parametrization of the linear xc response kernel $f_{xc}^{\text{hom}}(n, \omega)$ of the uniform gas.

(submitted to Physical Review Letters)
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Conventional Quantum Chemical Correlation Energy versus Density-Functional Correlation Energy

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Abstract

We analyze the difference between the correlation energy as defined within the conventional quantum chemistry framework and its namesake in density-functional theory. Both quantities are rigorously defined concepts; one finds that $E_c^{QC} \geq E_c^{DFT}$. We give numerical and analytical arguments suggesting that the numerical difference between the two rigorous quantities is small. Finally, approximate density functional correlation energies resulting from some popular correlation energy functionals are compared with the conventional quantum chemistry values.

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Scaling and virial theorems in current-density-functional theory

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Abstract

Starting from a constrained-search formulation of current-density-functional theory, we obtain rigorous scaling and virial relations for the kinetic, exchange and correlation energy functionals of electronic systems in strong magnetic fields. With the scaled density $n_\lambda(\mathbf{r}) \equiv \lambda^3 n(\lambda\mathbf{r})$ and the scaled *paramagnetic* current density $\mathbf{j}_\lambda(\mathbf{r}) \equiv \lambda^4 \mathbf{j}(\lambda\mathbf{r})$ the exchange energy functional $E_{\mathrm{x}}[n,\mathbf{j}]$ and the non-interacting kinetic energy functional $T_s[n,\mathbf{j}]$ satisfy $E_{\mathrm{x}}[n_\lambda,\mathbf{j}_\lambda] = \lambda E_{\mathrm{x}}[n,\mathbf{j}]$ and $T_s[n_\lambda,\mathbf{j}_\lambda] = \lambda^2 T_s[n,\mathbf{j}]$. The correlation energy functional satisfies the inequalities $E_{\mathrm{c}}[n_\lambda,\mathbf{j}_\lambda] \lessgtr \lambda E_{\mathrm{c}}[n,\mathbf{j}]$ for $\lambda \lessgtr 1$. Moreover, any homogeneously scaling functional $Q[n_\lambda,\mathbf{j}_\lambda] = \lambda^k Q[n,\mathbf{j}]$ obeys the relation:

$kQ + \int \mathrm{d}^3r\, n(\mathbf{r})(\mathbf{r}\nabla)[\delta Q/\delta n(\mathbf{r})] + \int \mathrm{d}^3r\, \mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)[\delta Q/\delta \mathbf{j}(\mathbf{r})] = 0.$

This relation, combined with the appropriate virial theorem in the presence of an external magnetic field, yields the following central theorems:

$E_{\mathrm{x}} + \int \mathrm{d}^3r\, n(\mathbf{r})(\mathbf{r}\nabla)[\delta E_{\mathrm{x}}/\delta n(\mathbf{r})] + \int \mathrm{d}^3r\, \mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)[\delta E_{\mathrm{x}}/\delta \mathbf{j}(\mathbf{r})] = 0$

and

$E_{\mathrm{c}} + \int \mathrm{d}^3r\, n(\mathbf{r})(\mathbf{r}\nabla)[\delta E_{\mathrm{c}}/\delta n(\mathbf{r})] + \int \mathrm{d}^3r\, \mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)[\delta E_{\mathrm{c}}/\delta \mathbf{j}(\mathbf{r})] = -T_{\mathrm{xc}},$

where $T_{\mathrm{xc}}[n,\mathbf{j}]$ is the difference of the interacting and the non-interacting kinetic energy functionals.

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Density-Functional Theory for Triplet Superconductors

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Abstract

The density-functional theory of superconductivity is extended to triplet superconductors and superfluid helium 3. We prove a Hohenberg-Kohn-type theorem for these systems and derive effective single-particle equations. The latter include exchange and correlations in a formally exact way and allow the treatment of both electronic and phonon-induced superconductivity. The relation of this approach to the Bogolubov-de Gennes mean-field theory and to phenomenological theories based on Ginzburg-Landau functionals is discussed.

(submitted to International Journal of Quantum Chemistry)
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A First Principles Investigation of Vacancy Oxygen defects in Si

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Abstract

Ab initio techniques are used to study vacancy oxygen complexes in Si. Substitutional oxygen is found to be an off-site defect in agreement with experiment. It possesses one high frequency O-related LVM at 788 cm^{-1}. The VO_2 defect has D_{2d} symmetry and only one O-related high frequency IR active mode at 807 cm^{-1}. The VO_3 defect has three high frequency IR active modes. The V_2O defect has one such LVM. These results provide strong support for the assignment of the 889 cm^{-1} (300 K) local vibrational mode to VO_2.

Keywords: *ab initio* theory, silicon, oxygen, vacancy, defect.

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A First Principles Study Of Ni Defects In Synthetic Diamond

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Abstract

We present the results of *ab initio* local density functional cluster calculations, using the AIMPRO program, performed on substitutional and interstitial Ni defects, and complexes of Ni with N and B.

Interstitial Ni^{+} (S=1/2) remains on the T_d site in contrast with results of previous calculations [2,3]. Ni^{++} (S=1) should be present in boron rich diamonds but as it has not been observed, we speculate that only substitutional Ni defects are found in diamond.

Substitutional Ni^{-} is found to be more stable, by around 1 eV, in an S=3/2 configuration than that with S=1/2, in agreement with experiment. The defect gives rise to a number of gap levels and could give rise to an optical transition around 1.4 and 2.6 eV.

Substitutional Ni^{+} (S=1/2) is found to have T_d symmetry at finite temperatures. A Jahn-Teller effect is expected for this defect, which could be trigonal, but is likely to be only observable at cryogenic temperatures. This defect is proposed for the NIRIM-1 EPR centre [5] that is found to have T_d symmetry at 25 K, but C_3v at 4 K, and observed in samples with low N concentration.

The trigonal $Ni_s^{+}B_s^{-}$ (S=1/2) complex is found to be stable. It gives rise to a number of states deep in the band-gap and an optical $e-a_1$ transition around 1.1 eV.

No hyperfine splitting due to B is expected. We propose this defect as responsible for the NIRIM-2 and the 1.4 eV optical centres.

The trigonal $Ni_s^- N_s^+$ (S=1/2) complex is stable and gives rise to an optical transition around 1.4 eV and may explain the 1.693 eV optical line seen in annealed N rich diamonds containing Ni [4].

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Keywords: *ab initio* theory, diamond, TM, nickel

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Interstitial H and the dissociation of C-H defects in GaAs

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Abstract

Local–density–functional calculations using a real–space cluster approach are used to model interstitial hydrogen in GaAs and the dissociation of the C–H and C–H^- complexes. The equilibrium site is found to be on a Ga–As bond axis for H^0 and H^+ and at a Ga anti–bonding site for H^-. It is also shown that a H_2 molecule is stable in interstitial space and has a lower energy than the two possible H_2^* defects and than widely separated single interstitial hydrogen atoms. The study of hydrogen in pure GaAs also yields the result that interstitial hydrogen is a negative–U defect. It is found that the energy barrier to the dissociation of the C–H complex is 1.8 eV, but that this is reduced to 0.9 eV for C–H^-. Comparison is made with recent experimental results and implications for current containing devices are discussed.

Keywords: C-H, dissocation, interstitial hydrogen, GaAs, *ab initio*

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Peculiarities of interstitial carbon and di-carbon defects in Si

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Abstract

The C_i and C_s-C_i defects in Si exhibit several unexplained properties. In the neutral charge state, the C_i defect possesses two almost degenerate vibrational modes suggesting a trigonal defect in disagreement with the C_{2v} symmetry deduced from several experiments. The B-form of the second defect is believed to consist of a Si interstitial, Si_i, located near a BC site between two C_s atoms, in apparent conflict with the results of PL experiments which show that the C-related vibrational modes are decoupled. The structure and vibrational modes of both defects are analysed using LDF cluster theory. The degeneracy of the modes of C_i is attributed to an almost D_{3h} structure, with a 3-fold axis along $[01\bar{1}]$. The modes of the di-carbon interstitial lead to a resolution of the long standing problem concerning the almost zero-shifts due to mixed isotopes in the 580 and 543 cm^{-1} local modes observed in PL studies.

Keywords: *ab initio* theory, carbon interstitials, silicon, vibrational modes

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Theory of the NiH_2 Complex in Si and the CuH_2 Complex in GaAs

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Abstract

Spin-polarised local density functional cluster calculations are carried out on substitutional Ni in Si and Cu in GaAs along with TM-H_2 complexes. The Jahn-Teller distortion for Ni in Si leads to a slight displacement along $\langle 100 \rangle$ in agreement with EPR experiments. Several models of NiH_2 are investigated and it is shown that one, with H located at anti-bonding sites to two of the Si neighbours of Ni, has the lowest energy and possesses H related local vibrational modes close to those reported for Pt-H_2. A similar structure is found for CuH_2 in GaAs. The electronic properties of the complexes are described in terms of the vacancy model of TM impurities.

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Theory of Si delta-doped GaAs

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Abstract

The insulating property of approx. 0.5 ML Si delta-doped GaAs is attributed to extended defects of self-compensated Si_{Ga}-Si_{As} pairs. The longitudinal and transverse optical modes of a chain and bilayer made from these pairs are calculated using first principles methods. The chain possesses a Raman active longitudinal mode at 470 cm^{-1} which drops to 465 cm^{-1}, when the chain is depleted of Si, and increases to about 500 cm^{-1} for Si rafts, ie (110) chains cross-linked by adjacent $(1\bar{1}0)$ chains. These results are in good agreement with recent Raman scattering studies which show a band increasing from 470 to 490 cm^{-1} when [Si] is increased from 0.5 ML to 2 ML. The theory also predicts three transverse branches, as well as a longitudinal resonant band, none of which have been reported so far.

Keywords: Si-delta doping, Si-Si chains, Raman scattering, *ab initio* theory

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Vacancy- and acceptor- H complexes in InP

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Abstract

It has been suggested that iron in InP is compensated by a donor, related to the 2316 cm^{-1} local vibrational mode and previously assigned to VH_4. Using *ab initio* local density functional cluster calculations, we find that the fully hydrogenated indium vacancy, VH_4, acts as a single shallow donor, and has a triplet vibrational mode at around this value, consistent with this assignment. We also analyse the other hydrogenated vacancies $VH_n, n = 1, 3$ and determine their structure, vibrational modes, and charge states. Substitutional Group II impurities also act as acceptors in InP, but can be passivated by hydrogen. We investigate the passivation of beryllium by hydrogen and find that the hydrogen sits in a bond centred site and is bonded to its phosphorus neighbour. Its calculated vibrational modes are in good agreement with experiment.

Keywords: *ab initio* theory, InP, donor, vacancy, hydrogen, defect, beryllium

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Ab initio full charge-density study of the atomic volume of α-phase Fr, Ra, Ac, Th, Pa, U, Np, and Pu

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Abstract

We have used a full charge density technique based on the linear muffin-tin orbitals method in first-principles calculations of the atomic volumes of the light actinides including Fr, Ra, and Ac in their low temperature crystallographic phases. The small deviations between the theoretical and experimental values along the series support the picture of itinerant $5f$ electronic states in Th to Pu. The increased deviation between theory and experiment found in Np and Pu may be an indication of correlation effects not included in present day local density approximations.

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Interlayer magnetic coupling: the torque method

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Abstract

We present ab-initio calculations of the interlayer exchange coupling between two, in general non-collinearly aligned magnetic slabs embedded in a non-magnetic spacer. Based on a surface Green's function formalism, two equivalent but formally and physically different approaches are examined and discussed. For the Co/Cu/Co(001) system we demonstrate the usefulness of the concept of infinitesimal rotations in order to calculate the coupling for a finite relative angle θ, in particular for $\theta = \pi$, between the corresponding spin directions in the magnetic slabs. The temperature and layer dependence of the interlayer exchange coupling is examined and the possibility for non-collinear coupling is investigated.

(submitted to Phys. Rev. B)
Preprint can be obtained from V. Drchal (vd@eecws7.tuwien.ac.at)

Interlayer magnetic coupling: effect of disorder in spacer

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Abstract

The influence of spacer randomness on the periods and the amplitudes of the oscillations of exchange coupling in magnetic multilayers is studied from first principles. The effect of disorder is treated within the coherent potential approximation. As a case study, results obtained for trilayers Co/$Cu_{1-x}M_x$/Co(001), where M=Ni, Pd, and Zn, are presented and discussed.

(submitted to JMMM)

Preprint can be obtained from J. Kudrnovský (jk@eecws7.tuwien.ac.at)

3d semicore-states in ZnSe, GaAs and Ge

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Abstract

We present the self-energy corrections for the semi-core states in ZnSe, GaAs and Ge within the GW approximation. Good agreement with experiment is found. To study the error trend in the local density eigenvalues which increases from ZnSe to Ge, we have also performed Slater transition state calculations. This increasing error can be understood in terms of the change of the occupation numbers of the orbitals and the Coulomb energies. We derived a simple formula to describe this increasing error.

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On the idea of a new quantum number in the cluster problem

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Abstract

It has recently been suggested that an exactly solvable problem characterized by a new quantum number may underlie the electronic shell structure observed in the mass spectra of medium-sized sodium clusters. We investigate whether the conjectured quantum number $3n+l$ bears a similarity to the quantum numbers $n+l$ and $2n+l$, which characterize the hydrogen problem and the isotropic harmonic oscillator in three dimensions.

(submitted to Phys. Rev. B)
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Supershells in metal clusters: Self-consistent calculations and their semiclassical interpretation

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Abstract

To understand the electronic shell- and supershell-structure in large metal clusters we have performed self-consistent calculations in the homogeneous, spherical jellium model for a variety of different materials. A scaling analysis of the results reveals a surprisingly simple dependence of the supershells on the jellium density. It is shown how this can be understood in the framework of a periodic-orbit-expansion by analytically extending the well-known semiclassical treatment of a spherical cavity to more realistic potentials.

(submitted to Phys. Rev. Lett.)
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Band Theory for Electronic and Magnetic Properties of α-Fe_2O_3

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Abstract

We report results of calculations that explain in the itinerant-electron picture magnetic and electronic properties of hematite, α-Fe_2O_3. For this we use the local approximation to spin-density functional theory and the ASW method incorporating spin-orbit coupling and noncollinear moment arrangements. The insulating character of the compound is obtained correctly and features in the density of states connected with Fe - O hybridization correlate well with experimental features seen in direct and inverse photoemission intensities. The total energy correctly predicts the experimentally observed magnetic order of the ground state, and, using total energies of different magnetic configurations, we can give a rough estimate of the Néel temperature. We also obtain a state showing weak ferromagnetism . The rate of change is calculated for the decrease of the insulating gap when an external magnetic field is applied.

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The Fermi Surface of UPd_2Al_3

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Abstract

The de Haas-van Alphen spectrum of UPd_2Al_3 is calculated and compared with the experimental spectrum for continuously varying directions of the magnetic field. The local approximation to spin-density functional theory is used for the self-consistent calculations treating the U 5f electrons as itinerant and including spin-orbit coupling. The amount of f-angular-momentum is obtained and visualized graphically for each sheet of the Fermi surface. The band-decomposed spin susceptibility, χ_0, is calculated for the states at the Fermi surface and the anisotropy of χ_0 is discussed.

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Spin and orbital polarized relativistic multiple scattering theory

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Abstract

A scheme is presented that allows to incorporate the orbital polarization (OP) mechanism into the Dirac equation for spin-polarized systems. This allows in a straightforward way to extend any band structure method accordingly – including those based on multiple scattering theory. The corresponding spin and orbital polarized relativistic version of the Korringa-Kohn-Rostoker-Coherent Potential Approximation (KKR-CPA) method has been implemented and applied to disordered bcc-Fe$_x$Co$_{1-x}$ alloys. Results for the spin and orbital magnetic moments as well as the spin-orbit coupling induced hyperfine fields are presented and discussed.

(submitted to Phys. Rev. B)

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Crucial role of the Lattice Distortion in the Magnetism of $LaMnO_3$

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Abstract

The stability of the A-type antiferromagnetic order and canted magnetic structure of $LaMnO_3$ perovskite is explained in the itinerant-electron picture based on the local-spin-density approximation. The lattice distortion plays a crucial role and determines behavior of both single-ion anisotropy, anisotropic *and* isotropic exchange interactions in this compound.

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Manuscripts available from: igor@jrcat.or.jp

A first-principles study of the magnetic hyperfine field in Fe and Co multilayers

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Abstract

We present *ab initio* calculations of the magnetic hyperfine field and magnetic moments in several Fe and Co multilayers $[Fe(Co)_2/Cu_6fcc-(001), FeCu(Ag)_5/fcc-(001), bcc-Fe/fcc-Ag_5(001), bcc-Fe_n/fcc-Au_5(001)(n=1,3,7), Co_k/Pd_lfcc-(111)(k(l)=1(5),2(4),3(3))andCo_2/Pt_mfcc-(111)(m=1,4,7)]$ as well as in bcc Fe and fcc (hcp, bcc) Co. The first-principles spin-polarized, relativistic linear muffin-tin orbital (SPRLMTO) method is used. Therefore, both the orbital and magnetic dipole contributions as well as the conventional Fermi contact term are calculated. Calculations have been performed for both in-plane and perpendicular magnetizations. The calculated hyperfine field and its variation with crystalline structure and magnetization direction in both Fe and Co are in reasonable agreement (within 10 %) with experiments. The hyperfine field of Fe (Co) in the interface monolayers in the magnetic multilayers is found to be substantially reduced compared with that in the corresponding bulk metal, in strong contrast to the highly enhanced magnetic moments in the same monolayers. It is argued that the magnetic dipole and orbital contributions to the hyperfine field are approximately proportional to the so-called magnetic dipole moment and the orbital moment, respectively. These linear relations are then demonstrated to hold rather well by using the calculated non-s electron hyperfine fields, orbital and magnetic dipole moments. Unlike in the bulk metals and alloys, the magnetic dipole moment in the multilayers is predicted to be comparable to the orbital moment and as a result, the magnetic dipole contribution to the hyperfine field is large. The anisotropy in the hyperfine field is found to be very pronounced and to be strongly connected with the large anisotropy in the orbital moment and magnetic dipole moment. The induced magnetic moments and hyperfine fields in the nonmagnetic spacer layers are also calculated. The results for the multilayers are compared with available experiments and previous nonrelativistic calculations.

(Phys. Rev. B (in press)); Preprints available from: g.y.guo@dl.ac.uk

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Non-collinear magnetism in Al-Mn topologically disordered systems

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Abstract

We have performed the first ab-initio calculations of a possible complex non-collinear magnetic structure in aluminium-rich Al-Mn liquids within the real-space tight-binding LMTO method. In our previous work we have predicted the existence of large magnetic moments in Al-Mn liquids [A.M. Bratkovsky, A.V. Smirnov, D. N. Manh, and A. Pasturel, Phys. Rev. B **52**, 3056 (1995)] which has been very recently confirmed experimentally. Our present calculations show that there is a strong tendency for the moments on Mn to have a non-collinear (random) order retaining their large value of about 3 μ_B. The d-electrons on Mn demonstrate a pronounced non-rigid band behaviour which cannot be reproduced within a simple Stoner picture. The origin of the magnetism in these systems is a topological disorder which drives the moments formation and frustrates their directions in the liquid phase.

(submitted to Europhys. Lett.)
The manuscripts are available from: alex.bratkovsky@materials.oxford.ac.uk

Adlayer core-level shifts of admetal monolayers on transition metal substrates and their relation to the surface chemical reactivity

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Abstract

Using density-functional-theory we study the electronic and structural properties of a monolayer of Cu on the fcc (100) and (111) surfaces of the late $4d$ transition metals, as well as a monolayer of Pd on Mo bcc(110). We calculate the ground states of these systems, as well as the difference of the ionization energies of an adlayer core electron and a core electron of the clean surface of the adlayer metal. The theoretical results are compared to available experimental data and discussed in a simple physical picture; it is shown why and how adlayer core-level binding energy shifts can be used to deduce information on the adlayer's chemical reactivity.

(Submitted to Phys. Rev. B)
REVTEX version can be obtained from: `vero@theo23.RZ-Berlin.MPG.DE`

Role of Self-Interaction Effects in the Geometry Optimization of Small Metal Clusters

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Abstract

By combining the Self-Interaction Correction (SIC) with pseudopotential perturbation theory, the role of self-interaction errors inherent to the Local Density Approximation (LDA) to Density Functional Theory is estimated in the determination of ground state and low energy isomeric structures of small metallic clusters. Its application to neutral sodium clusters with 8 and 20 atoms shows that the SIC provides sizeable effects in Na_8, leading to a different ordering of the low lying isomeric states compared with *ab-initio* LDA predictions, whereas for Na_{20}, the SIC effects are less pronounced, such that a quantitative agreement is achieved between the present method and *ab-initio* LDA calculations.

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The Effective Particle-Hole Interaction and the Optical Response of Simple Metal Clusters

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Abstract

Following Sham and Rice [L. J. Sham, T. M. Rice, Phys. Rev. **144** (1966) 708] the correlated motion of particle-hole pairs is studied, starting from the general two-particle Greens function. In this way we derive a matrix equation for eigenvalues and wave functions, respectively, of the general type of collective excitation of a N-particle system. The interplay between excitons and plasmons is fully described by this new set of equations. As a by-product we obtain - at least *a-posteriori* - a justification for the use of the TDLDA for simple-metal clusters.

(Submitted to Phys. Rev. B)

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Preprints from Center for Atomic-scale Materials Physics (CAMP)

- I. Stensgaard, E. Lægsgaard, and F. Besenbacher:
  The reaction of carbon dioxide with an oxygen-precovered Ag(110) surface
- P.T. Sprunger, Y. Okawa, F. Besenbacher, I. Stensgaard, and K. Tanaka:
  STM investigation of the coadsorption and reaction of oxygen and hydrogen on Ni(110)
- A.R.H. Clarke, J.B. Pethica, J.A. Nieminen, F. Besenbacher, E. Lægsgaard, and I. Stensgaard:
  Quantitative STM at atomic resolution: influence of forces and tip configuration
- P.W. Murray, I Stensgaard, E. Lægsgaard, and F. Besenbacher:
  Mechanisms of initial alloy formation for Pd on Cu(100) studied by STM
- P.M. Holmblad, J.H. Larsen, I. Chorkendorff, L.P. Nielsen, F. Besenbacher, I. Stensgaard, E. Lægsgaard, P. Kratzer, B. Hammer, and J.K. Nørskov:
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  Island shapes in homoepitaxial growth of Pt(111)
- P. Kratzer, B. Hammer, and J.K. Nørskov:
  Geometric and electronic factors determining the difference in reactivity of H_2 on Cu(110) and Cu(111)

More information can be obtained from helle@fysik.dtu.dk

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Presenting Other Human Capital and Mobility Projects

Report on research performed at Cineca, Bologne, Italy
supported by the EU Human Capital and Mobility Programme
ICARUS Scheme

Modelling of oxygen defects in silicon

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The European Union 'Human Capital and Mobility Programme' encompasses a range of schemes that share the common restriction that applicants should spend time working in a country other than their own. One such scheme is *ICARUS* [1], organised by CINECA, the Italian Universities' Central High Performance Computing (HPC) Facility [2].

ICARUS (*I*ntensive *C*omputing for *A*dvanced *I*nterdisciplinary *R*esearch of E*U*ropean *S*cientists) started in January 1994 and will finish in December 1996. It is designed to provide visitors with the training and resources necessary for research that requires supercomputing facilities. There are also many indirect benefits from such a scheme; the constant flux of researchers provides a fascinating insight into the way that other groups work, and allows comparison of many different software packages and applications. Finally the chance to stay in one of Italy's most central and cosmopolitan cities should not be missed.

CINECA is located in Casalecchio sul Reno [3], an industrial suburb of Bologne [4] in central Italy. It was originally set up in the early seventies by a small group of Italian universities, in recognition of the fact that high performance computing was too expensive to tackle individually. There are now 13 Universities in the consortium and CINECA acts as a central service for computing support, training and resources for the Italian Universities.

The resources at CINECA include a Cray C92/2128, Cray T3D (64 nodes; to be replaced with a larger T3E in 1996), IBM S/390-9672, VAX 6000-510, as well as many SGI and RS6000 machines. There is also a scientific visualisation laboratory and excellent network facilities to allow continued access from home sites after returning. All of the facilities are available to *ICARUS* visitors, along with training, support and documentation where required.

Details of the *ICARUS* scheme can be found on the CINECA World Wide Web site, including the necessary application forms and details of how to apply [1]. There are two other similar schemes at other supercomputing centres; the TRACS scheme at the Edinburgh parallel computing centre [5] and a scheme at CESCA/CEPBA in Barcelona [6]. All of these are designed to cover a broad spread of academic disciplines; in addition there are a number of single discipline centres including the European Molecular Biology Lab (EMBL) in Heidelberg, GEOMAR (Forschungszentrum für Marine Geowissenschaften), and the European Climate Computer Network including the Hadley Centre in Bracknell and the DKRZ in Hamburg [7].

I can thoroughly recommend the *ICARUS* scheme, as it was successful both in providing me with the resources I needed for my calculations, and broadening my knowledge of effective ways of utilising HPC resources. My previous HPC experience was primarily on the Cray at Edinburgh, and it was interesting to see the differences in approach between these two centres. The Cray T3D at CINECA has less nodes than Edinburgh and has a smaller workload, and due to its size and immanent replacement is used primarily for developmental work. My work on the Edinburgh Cray has been performed remotely, so there has been little opportunity for interaction with other users. At CINECA, however, discussion of various parallelisation strategies and different problem solving techniques proved extremely useful. I spent six weeks at Cineca during July and August, in order to use their Cray T3D to tackle the complex problem of oxygen diffusion in silicon.

Diffusion is an extremely important process in solids, affecting both their atomic structure and stability. However it is difficult to handle theoretically for several reasons. Firstly there are many possible channels for diffusion, including simple atomic exchange, interstitial or vacancy controlled diffusion, and diffusion catalysed by other impurities. Secondly, diffusion involves non-equilibrium structures, and requires the accurate determination of *saddle point structures* (structures possessing the highest energy along a particular diffusion path). This means that a lot of large calculations must be performed to examine even a relatively simple diffusion path, and workstations are prohibitively slow for such work.

The calculations were performed using the *Aimpro* code, a local density functional scheme applied to atomic clusters [8]. *Aimpro* has been developed at Exeter and Newcastle for over ten years [9], with successful application to a wide variety of molecular and semiconductor problems. Recent development of the code includes parallelisation and incorporation of the block algorithm SCALAPACK routines [10]. These routines take full advantage of massively parallel architectures. The code can run with comparable efficiency across a variety of platforms including parallel machines (such as the Cray T3D and IBM SP2), workstation clusters, and single workstations (eg SGI, IBM, and HP machines).

Oxygen in silicon has been an active area of research for over forty years. The main problem is to identify the structure and properties of oxygen aggregates, and determine the mechanism of interstitial creation. Oxygen is the most common impurity in commercial

Czochralski grown silicon, and forms many electrically active defects. The most important of these are *Thermal Donors*, that form during low temperature annealing from 300-500 °C [11]. In spite of intensive work, there has been no consensus about their structure.

Crucial to an understanding of how these defects form is a thorough investigation of how the defect atoms diffuse through the silicon lattice. Many of the oxygen related defects start to form at temperatures below 450 °C, however at these temperatures isolated interstitial oxygen does not diffuse. It has recently been suggested that oxygen may be able to diffuse much faster when travelling in pairs [12], which could diffuse at lower temperatures. If this was the case it would account for much of the unusual formation kinetics of oxygen defects.

Fast diffusing oxygen pairs would also have implications for low temperature formation of oxygen-vacancy complexes (such as VO_2) and would certainly affect our understanding of the oxygen diffusion mechanisms responsible for defect formation. Therefore I modelled the diffusion of a single oxygen interstitial and an interstitial oxygen pair.

Preliminary calculations using small clusters on the Cray gave a calculated energy barrier for single interstitial oxygen of 3.42 eV, and 2.14 eV for an oxygen interstitial pair. This supports the idea that an oxygen pair can diffuse at lower temperatures than a single oxygen interstitial. However the calculated single interstitial barrier is much higher than the experimental value of 2.54 eV, since the diffusion path requires a long range relaxation of lattice silicon atoms, which is not possible in the small cluster being used. Using the Cray T3D I was able to test this by examining different sizes of cluster (see Table 1). As the cluster size increases, the barrier drops gradually towards the experimental value. Work performed on 132 atom clusters since this project was completed is giving a calculated diffusion barrier for single interstitial oxygen of around 2.5 eV. Similar cluster size calculations are underway for the oxygen pair.

Table 1 : Effect of Cluster size on diffusion barrier for interstitial oxygen diffusion in silicon

Cluster	Number of Atoms	Energy Barrier (eV)
$Si_{11}H_{24}O$	36	3.424
$Si_{14}H_{30}O$	45	3.158
$Si_{35}H_{36}O$	72	2.969

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HIGHLIGHT OF THE MONTH

Ab-initio calculation of Giant Magnetoresistance in magnetic multilayers

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Introduction

Since the discovery of giant magnetoresistance (GMR) in magnetic multilayer systems (like Fe/Cr or Co/Cu) [1, 2] several experimental and theoretical studies have been carried out to elucidate the microscopic origin of the phenomenon. Here, *ab initio* calculations of the electronic structure and of the electron scattering are of great interest.

The GMR effect occurs when successive ferromagnetic layers exhibit anti-parallel magnetization. The application of an external magnetic field brings the magnetization of the ferromagnetic layers into alignment and causes a decrease of resistivity (Fig. 1) for both current-in-plane (CIP) and current-perpendicular-to-plane (CPP) geometries (see Fig. 2).

Most theories [4, 12, 10, 9, 22, 11] try to explain the GMR by spin-dependent scattering at interfaces or bulk defects but neglect the electronic structure of the multilayer system. Attempts to include the electronic structure have been made by several authors [16, 3, 21,

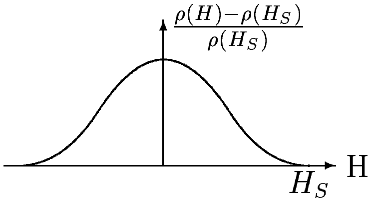

Figure 1: Giant magnetoresistance. The resistivity is maximum when the magnetic moments of successive ferromagnetic layers are antiparallel. It drops off as the applied field aligns the magnetic moments H_S, denoted by the right and left diagrams for positive and negative fields, respectively.

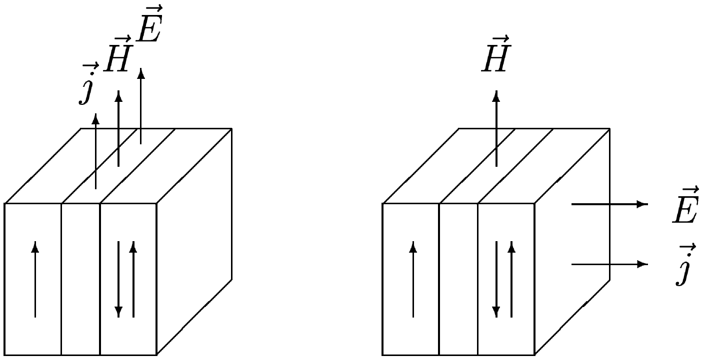

Figure 2: Geometrical arrangements of current density **j**, electrical field **E** and magnetic field **H** in CIP and CPP measurement of GMR.

23]. All calculations predict a strong influence of the electronic structure of the multilayer on the GMR.

The GMR in magnetic multilayers is defined as

$$\mathrm{GMR} = \frac{\sigma^P}{\sigma^{AP}} - 1, \tag{1}$$

where σ^P and σ^{AP} are the conductivities of the multilayer for parallel and anti-parallel alignment of successive ferromagnetic layer magnetization, respectively. Experimentally, one can be sure that parallel alignment is achieved, in view of the marked transition from strong to weak magnetic field dependence of the conductivity at the saturation field (see Fig. 1).

Electronic structure of the multilayer

Our considerations focus on (100) oriented Fe_mCr_n layer sequences (m monolayers of Fe followed by n monolayers of Cr), where the Fe layers are intrinsically ferromagnetic and the Cr layers are intrinsically antiferromagnetic. *Ab initio* electronic structure calculations have been performed using spin-density functional theory for initially parallel and antiparallel spin configurations of subsequent Fe layers [23].

Starting from the bandstructure E_k^σ of the situation, that we have just addressed, potential scattering causes transitions from a state k into a state k' of the multilayer system. The scattering can be caused by impurity atoms in the ferromagnetic or in the nonmagnetic spacer layer. The scattering is described by spin-dependent relaxation times τ^σ which are different for majority and minority electrons depending on the type of scatterer. The spin anisotropy ratio $\beta = \tau^\uparrow/\tau^\downarrow$ is a direct measure. $\beta < 1$ means strong scattering of the majority electrons and for $\beta > 1$ the minority electrons are strongly scattered.

Transport theory

Transport is described within the quasiclassical theory solving the Boltzmann equation in relaxation time approximation. Consequently, the conductivity tensor becomes

$$\hat{\sigma}^\sigma = e^2 \tau^\sigma \sum_k \delta(E_k^\sigma - E_F)\, \mathbf{v}_k^\sigma\, \mathbf{v}_k^\sigma. \tag{2}$$

The integration is performed over the Fermi surface of the parallel configuration of the layered system. Summation of the two currents yields the total conductivity

$$\hat{\sigma}^P = \hat{\sigma}^\uparrow + \hat{\sigma}^\downarrow. \tag{3}$$

In the anti-parallel configuration the electronic states are spin degenerate, and the conductivity becomes

$$\hat{\sigma}^{AP} = 2\, e^2 \tau^{AP} \sum_k \delta(E_k^{AP} - E_F)\, \mathbf{v}_k^{AP}\, \mathbf{v}_k^{AP}. \tag{4}$$

Assuming that the layered system is grown in the z direction, CIP corresponds to the xx or yy component of the conductivity tensor and CPP to the zz component in Eqs. 2 and 4. τ^{AP}, the relaxation time in the anti-parallel configuration, can be obtained by summation of the scattering operators. For equal concentration of defects in adjacent ferromagnetic layers, the relaxation time is then given by

$$\frac{1}{\tau^{AP}} = \frac{1}{2}\,\left(\frac{1}{\tau^\uparrow} + \frac{1}{\tau^\downarrow}\right). \tag{5}$$

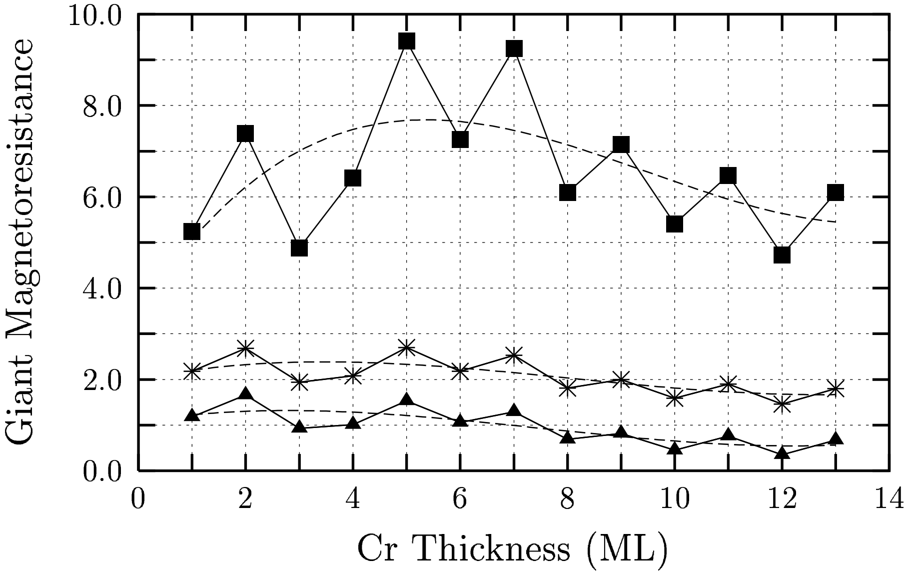

Figure 3: Calculated CIP-GMR for Fe_3Cr_n versus Cr layer thickness $n = 1, 13$. The results assuming Cr defects in the Fe layers are indicated by squares ($\beta = 0.11$). Stars mark the results for spin-independent relaxation times $\beta = 1$ and triangles for $\beta = \beta_{min}$.

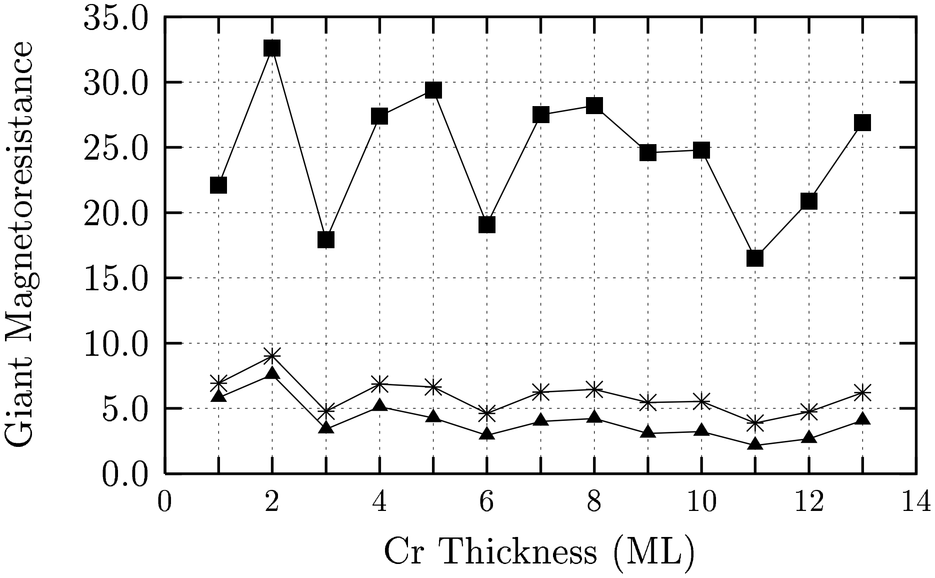

Figure 4: Calculated CPP-GMR for Fe_3Cr_n versus Cr layer thickness $n = 1, 13$. The results assuming Cr defects in the Fe layers are indicated by squares ($\beta = 0.11$). Stars mark the results for spin-independent relaxation times $\beta = 1$ and triangles for $\beta = \beta_{min}$.

Results

The simplest situation occurs, when all the scattering centers are localized in the antiferromagnetic Cr layers (for example Fe impurities).

In this case the lifetimes τ^σ for both spin directions must be equal since the spin up wavefunction amplitudes of one half of the Cr atoms is equal to the spin down wavefunction amplitudes of the other half. This corresponds to $\beta = 1$. Eq. 5 now implies $\tau^{AP} = \tau^{\uparrow} = \tau^{\downarrow}$. Hence the lifetime completely disappears from the GMR expression

$$\mathrm{GMR} = \frac{\sum_\sigma \sum_k \delta(E_k^\sigma - E_F)\, v_{k\,\mu}^\sigma\, v_{k\,\mu}^\sigma}{2\ \sum_k \delta(E_k^{AP} - E_F) v_{k\mu}^{AP}\ v_{k\mu}^{AP}} - 1. \tag{6}$$

Here, the GMR is fully determined by the Fermi surface and Fermi velocities as functions of the magnetization configuration. Hence it is a pure bandstructure effect. The obtained GMR values are about 200% in CIP and 700% in CPP (stars in Fig. 3 and 4), which is in agreement with the experimentally obtained maximum CIP-GMR (220%) for ultrathin Fe layers [20].

Simplifying Eq. 6 for further discussion of the origin of GMR leads to

$$GMR = \frac{\sum_\sigma N^\sigma(E_F) v_\mu^{\sigma 2}}{N_{AP}(E_F)\ \ v_\mu^{AP2}} - 1 \tag{7}$$

with the density of states of the superlattice for parallel alignment

$$N_P(E_F) = \sum_\sigma\ N^\sigma(E_F) = \sum_\sigma \sum_k \delta(E_k^\sigma - E_F) \tag{8}$$

and for anti-parallel alignment

$$N_{AP}(E_F) = 2\ \sum_k \delta(E_k - E_F). \tag{9}$$

v_μ^σ and v_μ^{AP} are Fermi surface averages of the Cartesian components of the velocity for parallel

$$v_\mu^\sigma \ = \ \sqrt{\frac{\sum_k \delta(E_k^\sigma - E_F)\, {v_{k_\mu}^\sigma}^2}{\sum_k \delta(E_k^\sigma - E_F)}} \tag{10}$$

and anti-parallel alignment

$$v_\mu^{AP} \ = \ \sqrt{\frac{\sum_k \delta(E_k^{AP} - E_F)\, v_{k_\mu}^{AP2}}{\sum_k \delta(E_k^{AP} - E_F)}}. \tag{11}$$

The densities of states in the parallel and anti-parallel configuration (Fig. 5) are of the same order and they oscillate in phase with the Cr layer thickness, that is, they do not account for the 200% CIP-GMR and 700% in CPP-GMR (Fig. 3 and 4). Obviously, GMR is originated by the differences in the Fermi velocities in the parallel and anti-parallel configurations (Fig. 6).

The spin dependence of the relaxation time ($\beta \neq 1$) due to scattering centers in the ferromagnetic layers (Cr impurities in Fe layers, for example) leads to modifications.

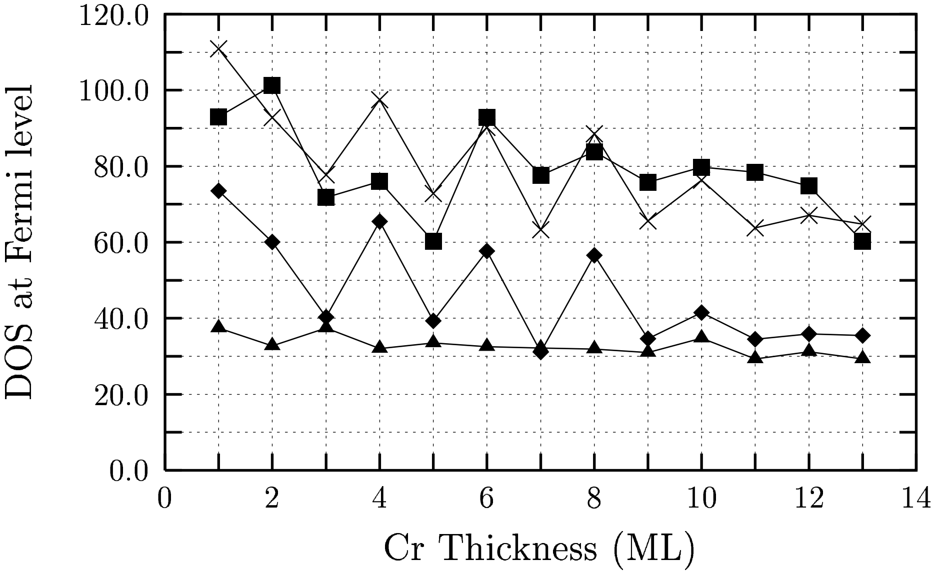

Figure 5: $N_P(E_F)$ (squares) and $N_{AP}(E_F)$ (times) of Fe_3Cr_n superlattices versus Cr layer thickness in arbitrary units. The spin-projected densities of states of $N_P(E_F)$ are marked as follows: $N^{\uparrow}(E_F)$ (diamonds) and $N^{\downarrow}(E_F)$ (triangles) [13].

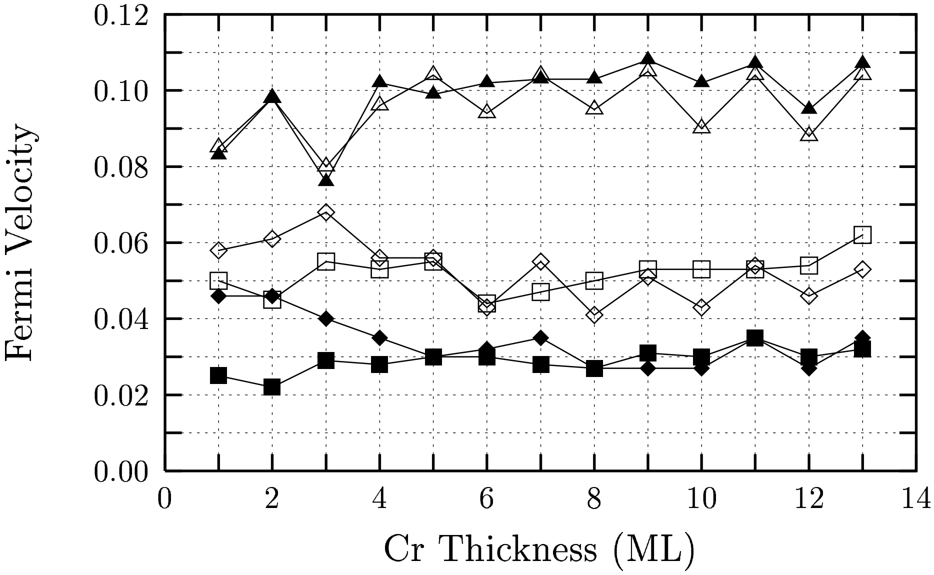

Figure 6: Fermi surface averages of the velocity components. Open symbols indicate v_x and full symbols v_z. Diamonds mark the velocity of majority electrons, triangles the velocity of minority electrons and squares the velocity in the anti-parallel aligned configuration [13].

GMR is now to be calculated via Eq. 1, 2 and 4. Under the assumption that the extension of the impurity is small compared to the layer thickness, the scattering properties are described by the spin-dependent relaxation times calculated for the Cr impurities in Fe [14, 15]. For this case $\beta = 0.11$, that is, the majority electrons are scattered strongly at a Cr defect and the minority electrons are just weakly scattered as they pass the defect.

The results assuming Cr defects located in the Fe layers lead to a GMR of about 600% in CIP (squares in Fig. 3) and 2500% in CPP (squares in Fig. 4) which is larger than the experimental results [8, 6, 18, 7]. The anisotropy β obtained in [14, 15] for a variety of defects scatter from 0.1 to 10. Therefore, GMR is discussed as a function of β in relaxation time approximation. If only one type of scatterer is included, GMR becomes a minimum for

$$\beta_{min} \;=\; \frac{\tau^{\uparrow}}{\tau^{\downarrow}} = \sqrt{\frac{\sum_k \delta(E_k^{\downarrow} - E_F)\, v_{k\mu}^{\downarrow\,2}}{\sum_k \delta(E_k^{\uparrow} - E_F)\, v_{k\mu}^{\uparrow\,2}}}. \tag{12}$$

That is, GMR can be enhanced or reduced by spin-dependent impurity scattering. The results for $\beta = \beta_{min}$ are shown in Fig. 3 and 4 (triangles).

Finally, we discuss the combination of alternating Fe layers with Cr defects ($\beta = 0.11$) and with Cu defects ($\beta = 3.68$). For the sake of simplicity, equal concentration is assumed. The relaxation times are in parallel configuration

$$\frac{1}{\tau^{\sigma}} = \frac{1}{2}\,(\,\frac{1}{\tau_{Cr}^{\sigma}} \;+\; \frac{1}{\tau_{Cu}^{\sigma}}\,), \tag{13}$$

and in anti-parallel configuration

$$\frac{D_{\uparrow}^{+} + D_{\uparrow}^{-}}{\tau^{\uparrow}} = (\,\frac{D_{\uparrow}^{+}}{\tau_{Cr}^{+}} \;+\; \frac{D_{\uparrow}^{-}}{\tau_{Cu}^{-}}\,), \tag{14}$$

and

$$\frac{D_{\downarrow}^{+} + D_{\downarrow}^{-}}{\tau^{\downarrow}} = (\,\frac{D_{\downarrow}^{-}}{\tau_{Cr}^{-}} \;+\; \frac{D_{\downarrow}^{+}}{\tau_{Cu}^{+}}\,), \tag{15}$$

respectively where the superscripts $+, -$ correspond to majority and minority electrons. D_{σ}^{+} and D_{σ}^{-} is the local spin-dependent density of states in a ferromagnetic layer where spin-σ electrons are majority or minority electrons, respectively. In the considered configuration the factors have been set to unity. The conductivity in the anti-parallel state including both defects is given by

$$\hat{\sigma}^{AP} = e^2(\tau^{\uparrow} + \tau^{\downarrow}) \sum_k \delta(E_k^{AP} - E_F)\, \mathbf{v}_k^{AP}\, \mathbf{v}_k^{AP}. \tag{16}$$

The results are shown in Fig. 7. The main message from this calculation is that the GMR can be reduced drastically or even change sign, if scatterers with different spin anisotropy are combined. (If they would be located in the same layer they would merely

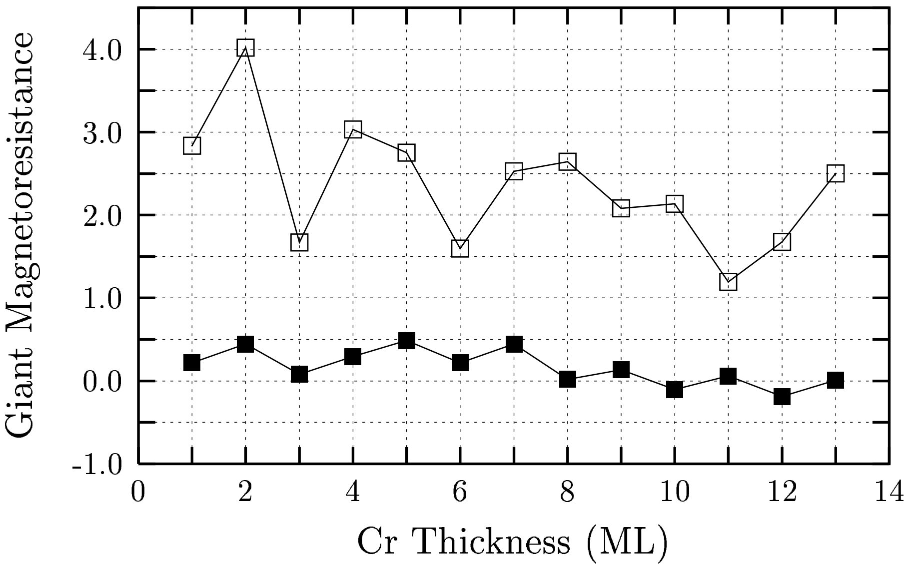

Figure 7: Calculated GMR for Fe_3Cr_n with Cr and Cu defects in adjacent Fe layers in CIP (closed squares) and CPP (open squares). For $n \geq 10$ the inverse GMR is obtained.

act as an effective scattering potential.) One should note that in Fig. 7 the inverse effect occurs in CIP but not in CPP. Experimentally, the inverse effect was obtained for $Fe/Cr/Fe/Cu/Fe/Cu$ multilayers [5], as well as in $Fe_{1-x}V_x/Au/Co$ multilayers [19], both in CIP geometry.

Generally, it should be noted that CPP-GMR for comparable scattering is always larger than CIP by a factor of about 4 in agreement with experimental results [7]. This factor stems from the difference of the Fermi velocity components in plane and perpendicular to the plane, and it finds its natural explanation in the fact that the carriers with large momentum components in direction of the current are more influenced by the superstructure in CPP.

Moreover, GMR (Fig. 3, 4, 7) shows characteristic variations with layer thicknesses. On Fig. 7 these variations are reminiscent of experimentally found oscillations [17].

Summary

In conclusion, we have shown that GMR, under the assumption of a coherent multilayer system and a spin-independent impurity scattering, is determined by the changes of the electronic structure as a function of the magnetization direction. Spin-dependent impurity scattering can enhance or reduce the effect. The combination of impurities with different spin anisotropy can in particular cause the inverse GMR.

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Announcement

UNIVERSITY OF OXFORD–DEPARTMENT OF MATERIALS
MATERIALS MODELLING LABORATORY

BOND–ORDER POTENTIALS WORKSHOP

18 AND 19 MARCH 1996

The realistic atomistic simulation of materials requires the development and application of O(N) methods that avoid the crippling N^3 constraint of matrix diagonalisation for finding the electronic structure and hence the energy of a system.

This two-day workshop presents the background theory and concepts behind the novel Bond Order Potentials (BOPs) which allow the Tight Binding (TB) energy to be expressed exactly as a rapidly convergent many-atom expansion. The BOP approach has the advantage over other O(N) density matrix methods in that it is equally applicable to both metals and semiconductors, and it is naturally parallelisable.

The nature of the BOP computer codes will be described and a hands-on afternoon session will give workshop attendees experience in simulationg a wide range of materials from hydrocarbon molecules through to bulk semiconducsctors and intermetallics.

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OXYGEN '96

Early Stages of Oxygen Precipitation in Silicon
NATO Advanced Research Workshop
26th - 29th March 1996

University of Exeter, U.K.

Co-sponsored by the University

Objectives:

Topics to be covered include: Progress and problems involved with the early stage of oxygen precipitation in silicon; oxygen diffusion and clustering; oxygen-light element interactions especially H, C and N; oxygen-TM defects; oxygen-vacancy and interstitial complexes; thermal and new donors; theoretical modelling of oxygen defects and processes. A major aim is to bring theoretical modelling groups together with experimental ones to promote cross-fertilisation of ideas.

Speakers Include:

C. A. J. Ammerlaan, P. Deák, S. Estreicher, C. Ewels, U. Gosele, J. L. Lindström, V. P. Markevich, R. C. Newman, B. Pajot, J. M. Spaeth, M. Stavola, M. Suezawa, K. Sumino, G. D. Watkins, E. R. Weber, J. Weber

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Accomodation and Fees:

Full board is available from the evening of Monday March 25, 1996, through to Friday lunchtime on March 29th for 266 pounds sterling, including reception, conference dinner and an excursion. Some contribution to the travel and accommodation costs may be made subject to the regulations of NATO.

Proceedings:

Will be published in the NATO ASI series.

Registration:

World Wide Web site: `http://newton.ex.ac.uk/NATO/` It is possible to register directly using the World Wide Web, or else complete the form enclosed below and return to `ewels@excc.ex.ac.uk` or `jones@excc.ex.ac.uk`

Travel:

The University is located in Exeter, the beautiful county town of Devon in the South West of England. It can be reached by train from London (Paddington or Waterloo - 2:30 hrs). Delegates from London airport (Heathrow) should take the airport bus to Reading and then the train to Exeter (2 hrs). Alternatively coaches run from London (Victoria) or Heathrow directly to Exeter (3 hrs). The University is a few minutes taxi-ride from either the train or coach station.

Organising Committee:

Dr. R. Jones - Department of Physics, University of Exeter, U.K. Prof. P. Deák - Department of Atomic Physics, Technical University, Budapest, Hungary. Prof. S. Estreicher - Max Planck Institute, Stuttgart, Germany. C. Ewels - Department of Physics, University of Exeter, U.K.

OXYGEN '96 Registration Form follows.

OXYGEN ’96 Registration Form

General Details:

Title: [ ]Prof [ ]Dr [ ]Mr [ ]Mrs [ ]Ms Other ___________
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Do have any special requirements? (Diet, disability, etc.)
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Plese quote the cost of economy travel between London (Heathrow or Victoria) and your home base:
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I would like to submit a poster [ ] Yes [ ] No
Title: ____
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Abstract: This can also be sent directly by e-mail, preferably in
          LaTeX/ReVTeX format, to ewels@excc.ex.ac.uk
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Ψ_k Network Conference

organized by the European Union HCM network

"Ab initio (from electronic structure) calculation of complex processes in materials"

Schwäbisch Gmünd, September 18-21, 1996

Second Circular and call for suggestions

Scientific Program

Methods

- **Quantum Monte Carlo Calculations**
- **New developments in Muffin-tin and Pseudopotential techniques**
- **Density Functional Molecular Dynamics simulation: methods and applications**
- **Beyond the Local Density Approximation**
- **Quasiparticles**
- **Solving the Bogolubov-de Gennes Equations**
- **Approximate Methods for large systems**
- **Parallel Algorithms (Parallelisation)**

Applications to all aspects of Condensed Matter and Materials Science including:

- Electron spectroscopies
- Novel superconductors
- Magnetic multilayers

- Oxide/metal interfaces
- Reactions at surfaces
- Semiconductor heterostructures and quantum wires
- Carbon structures
- Molecular materials

The conference is open to anyone interested. The expected attendance is 300. All abstracts will be accepted, either as a contributed talk or as a poster, subject to the limitation that each participant presents at most one talk or poster.

Suggestion Form for invited speakers and symposia

Members of the network and external keypersons are asked to suggest a plenary speaker as well as a topic, two speakers, and a chairperson for a symposium. We plan to have 8 plenary sessions and 8-12 symposia running three in parallel.

Accompaning this 2^{nd} circular is a suggestion form either in print or as electronic mail (LaTeX file form.tex plus LaTeX style psik.sty). Only forms arriving by **January 15th 1996** will be considered. We therefore recommend the return of the completed form.tex file via electronic mail to psik@radix2.mpi-stuttgart.mpg.de.

Timetable

Jan 15	1996	Deadline for suggestions.
Apr	1996	Third circular including details about symposia and invited speakers.
May	1996	Deadline for the submission of abstracts and registration.
Jun	1996	Final programme.
Sep	1996	Conference.

Location: Schwäbisch Gmünd (Germany)

Schwäbisch Gmünd is located in south-west Germany 50 kilometers east of Stuttgart, the capital of the state of Baden-Württemberg. It is easily accessible by public transport from Stuttgart and from Stuttgart international airport.

The conference will be held at the Stadtgarten conference center which is within walking distance from most of the hotels. Schwäbisch Gmünd is a lovely old town with a population of 60,000 and with a history dating back to the Roman Empire in the 2nd century. In the 12th century it became the first of several imperial towns founded by the Hohenstaufen dynasty to protect their empire. Many original old buildings show the transition of the former Free Imperial City from Gothic through Renaissance to Baroque and the coexistence of 19th century palatial grandeur with contemporary architecture.

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O.K. Andersen, A. Burkhardt, O. Jepsen,
C. Irslinger, G. Schmidt, Z. Szotek, W.M. Temmerman

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Further Information

Up to date information may be obtained from the World-Wide-Web Conference server at **http://radix2.mpi-stuttgart.mpg.de/hcm.html** .

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