Ψ_k Newsletter

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

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Editor: Z. (Dzidka) Szotek
E-mail: psik-coord@dl.ac.uk

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1 Editorial

In this *Newsletter* in the **General News** section we write about the Max Born Medal and Prize and this year's recipient, professor Volker Heine from Cambridge University, UK. The **TMR1** and **RTN** sections contain reports on recent workshops, including abstracts of presented talks. As always abstracts of newly submitted papers are placed in the usual **Abstracts** section. In the **RTN**, **TMR2** and **ESF** sections readers will find a few workshop/conference announcements. Meetings organized without financial sponsorship of the Psi-k Network are announced in the **General Workshop/Conference Announcements** section. The **ESF** section, apart from one workshop report, contains also reports on collaborative visits. Information on available postdoctoral and Ph. D. positions can be found in the **General Job Announcements** section. In the **Book Announcements** section we advertise a book by K.N. Shrivastava (*University of Hyderabad, India*) on **"Superconductivity: Elementary Topics"**. The *Newsletter* is finished with the scientific highlight of the month by M. Woods, P. Strange (*Keele University, UK*), A. Ernst (*Max-Planck-Institute Halle, Germany*), and W.M. Temmerman (*Daresbury Laboratory, UK*) on **"Real-space relativistic spin-polarized photoemission"**. 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 2001 workshops and hands-on courses. In these pages you can also find information on how to apply for funding to make collaborative visits.

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

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

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

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

2 General News

2.1 2001 Max Born Medal and Prize

Volker Heine (Cambridge University, UK) receives Max Born Medal and Prize

Volker Heine, the driving force behind the Psi-k Network, has been awarded the 2001 Max Born Medal and Prize *"For his pioneering theoretical and computational studies of the electronic structure of solids and their application to physical properties, including his recent contributions to the development of a new field of "mineral physics""*.

The Max Born Medal and Prize:

History:

The Institute of Physics (UK) and the German Physical Society instituted this award in 1972 to commemorate Max Born who died in 1970. Like the Holweck Medal and Prize, the award is intended both to commemorate the name of the physicist and to cement the relationship between the two institutions. The award is made alternately by the Councils of one of the two societies to a physicist selected from a list of nominees submitted by the other.

Terms:

The award shall be made for outstanding contributions to physics in even dated years to a German physicist and presented in England and in odd dated years to a British or Irish physicist and presented in Germany. The award consists of a silver medal and is accompanied by a prize of £750 and a certificate.

About the medallist for 2001:

"Why don't you go over to the low-temperature physics group and see if you can make yourself useful", was the suggestion made to Volker Heine by Sir Nevill Mott for his PhD when Heine came to the UK from New Zealand. Since then most of Heine's work has been on the theory and computation of the electronic structure of solids. It has covered metals, surfaces, alloys, magnetism and minerals and has been characterized by the interpretation of experimental results. The advent of the EDSAC I electronic computer added a new dimension in relating theory and

experiment. Heine used this computer between 1954 and 1956 for his PhD work to calculate the electron band structure of aluminium, for which data were just being obtained.

In the 1960s Heine worked with Igor Abarenkov and Alex Animalu in developing "pseudopotentials" for 25 elements that remained widely used for a decade. The simple description that these pseudopotentials yield for the interaction of the outer conduction or bonding electrons with the atoms in a solid made many calculations of structures and properties possible.

Following a breakthrough in 1978, accurate "computer experiments" have allowed scientists to model all of the bonding electrons in a solid using quantum mechanics. With colleagues Richard Needs and Mike Payne in Cambridge, Heine has championed this development ever since and has led European collaboration in the field.

In around 1980, Desmond McConnell drew him into applying theoretical physics and computer simulation to problems in silicate minerals. In partnership with Ekhardt Salje and Martin Dove, he helped to develop this work into a new field of "mineral physics". (After December 2000 issue of Physics World)

In the UK, and indeed in Europe generally, Volker Heine established an approach to solid state physics in which the fundamental quantum mechanical equations were solved in a physical, yet precise, way which made contact with real systems. This has had enormous ramifications not only in physics but also in materials science, surface science, metallurgy, mineralogy and chemistry. Moreover, his contributions reach far beyond his own research. He is an excellent teacher and has established a whole school of condensed matter theory which extends through this country and abroad. He has always maintained and advocated strong links with groups throughout Europe, the USA and Japan. For many years he has been particularly closely involved with Max-Planck-Institute in Stuttgart. In recent years, as all our readers are aware of, he has established the Psi-k Network to raise the profile and quality of electronic structure studies throughout Europe and particularly the smaller and less developed countries. The tremendous impact this Network has had for computational physics in Europe cannot be overstated.

Volker Heine has published over 200 research papers, several review articles and one text book (on the use of group theory). Many papers concern the theory and calculation of the electronic structure of solids including surfaces, with particular emphasis on aspects of interatomic bonding and structure.

Volker Heine had and has the talent to pose questions and to describe results so that he has always stimulated most fruitful discussions in the scientific community.

We congratulate him on this award and wish him all the best for the future.

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Reports on Workshops/Conferences

3.1.1 Report on XRMS2000 Workshop

International Workshop on X-ray Spectroscopy for Magnetic Solids 2000 (XRMS2000)

Berlin, Saturday 9-th December 2000

Organizers: K. Starke, FU Berlin email: starke@physik.fu-berlin.de
H. Ebert, LMU Munich email: hubert.ebert@cup.uni-muenchen.de

The workshop was held at the Physics Department of the Freie Universität (FU) Berlin, following the annual user meeting of BESSY II, the new synchrotron facility at Berlin Adlershof. One of the central aims of the meeting was to bring together experimental and theoretical groups working in the field of X-ray spectroscopy of magnetic materials. Although there was some emphasis on magnetic scattering and microscopy techniques, the various invited contributions reflected the many recent activities in this wide field in a relatively complete way. All talks were followed by very lively discussions that were continued during the breaks and in particular during the poster session. The interesting contributions, e.g. on X-ray magneto-optics, to this session nicely complemented the topics covered by the oral talks.

According to the comments by many participants, the workshop was very successful and fruitful. We hope we can document this by the proceedings that will appear in **Applied Physics A** and will reflect some selected contributions to the workshop. (see also: http://www.physik.fu-berlin.de/ starke/xrms2000)

XRMS2000 list of participants

Baberschke Klaus, FU Berlin, Germany
Bansmann Joachim, Universität Rostock, Germany
Bayer Andreas, Universität Würzburg, Germany
Benea Diana, Universität München, Germany

Braicovich Lucio, Polytechnico, Italy
Brewer William D., FU Berlin, Germany
Brooks Mike, FZ Karlsruhe, Germany
Brouder Christian, Jussieu, France
Dartyge Elisabeth, Lure, France
Dudzik Esther, Hahn-Meitner Institut, Germany
Dürr Hermann, FZ Juelich, Germany
Eberhardt Wolfgang FZ Juelich, Germany
Ebert Hubert, Universität München, Germany
Eimueller Thomas, Universität Würzburg, Germany
Fauth Kai, Universität Würzburg, Germany
Frota-Pessôa Sonia, University Sâo Paulo, Brazil
Geissler Jochen, Universität Würzburg, Germany
Getzlaff Matthias, Universität Hamburg, Germany
Giorgetti Ch., Lure, France
Goedkoop Jeroen, University of Amsterdam
Goering Eberhard, Universität Würzburg, Germany
Grigoriev Alexeji, FU Berlin, Germany
Heigl Franziskus, FU Berlin, Germany
Hessler Markus, Universität Würzburg, Germany
Hill John, Brookhaven Natl. Lab., U.S.A.
Horn Karsten, FHI Berlin, Germany
Jaouen Nicolas, Grenoble, France
Jensen Peter, Hahn-Meitner Institut, Germany
Kaindl Günter, FU Berlin, Germany
Kirchner Thomas, Universität Halle, Germany
Krupin Oleg, FU Berlin, Germany
Kuch Wolfgang, MPI-Halle, Germany
Lindner Jürgen, FU Berlin, Germany
Minar Jan, Universität München, Germany
Müller Norbert, Universität Bielefeld, Germany
Münzenberg Markus, Göttingen, Germany
Muschiol Uwe, IFW-Dresden, Germany
Ney Andreas, FU Berlin, Germany
Oppeneer Peter M., IFW-Dresden, Germany
Ott Holger, FU Berlin, Germany
Perlov Alexander, Universität München, Germany
Poulopoulos Panagiotis, FU Berlin, Germany
Prieto Jose Emilio, FU Berlin, Germany
Rüdt Christoph, FU Berlin, Germany
Scherz Andreas, FU Berlin, Germany
Scholl Andreas, Lawrence Berkeley Natl. Lab., U.S.A.
Schreyer Andreas, Universität Bochum, Germany

Schuessler-Langeheine Christian, FU Berlin, Germany
Starke Kai, FU Berlin, Germany
Strange Geoffry, University of Keele, GB
Tsetseris Leonidas, MPI-Stuttgart, Germany
van der Laan Gerrit, Daresbury Labs., GB
Vyalikh Denis, FU Berlin, Germany
Wende Heiko, FU Berlin, Germany
Weschke Eugen, FU Berlin, Germany
Wilhelm Fabrice, FU Berlin, Germany
Wortmann Gerhard, Universität Paderborn, Germany
Zabel Hartmut, Universität Bochum, Germany

Abstracts of invited speakers

Theoretical description of the Fano-effect in the angle integrated valence band photoemission of paramagnetic solids

J. Minár and H. Ebert
Department Chemie/ Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 München, Germany

Abstract

A theoretical description of the Fano-effect in the angle integrated valence band photoemission of paramagnetic solids is presented that is based on the one-step-model of photoemission and relativistic multiple scattering theory. Applications to Cu and Ag led to a very satisfying agreement with recent experimental data that show the Fano-effect, i.e. a finite spin-polarisation for the spectra is found for excitation with circularly polarised radiation. As can be demonstrated by model calculations this finding is caused by the presence of the spin orbit coupling. To allow for a more detailed discussion of the spectra a simplified description of the Fano-effect is presented that treats spin orbit coupling as a perturbation. A similar effect was found also for the 3d core-level photoemission specta of paramagnetic Ag and our results will be shown as well.

Magnetic Circular Dichroism in Soft X-Rays Resonant Inelastic Scattering

L. Braicovich
INFM – Dipartimento di Fisica del Politecnico
Piazza Leonardo da Vinci 32 – 20133 Milano – Italy

Abstract

We discuss the information one can obtain in the measurements of Magnetic Circular Dichroism in Soft X-Rays Resonant Inelastic Scattering. In particular the goal is the discussion of the information one can add to those obtained from absorption Magnetic Circular Dichroism (MCD). This is done by presenting both published and unpublished results in three fields which are critically presented:

(i) the experiments in which the incidence of the photon beam is nearly parallel to the magnetisation with the measurement, at selected excitation energies, of the energy distribution of the photons emitted at an angle. Final states with valence excitation are considered. Results on Fe-Co alloys are presented showing that the method is very convenient in the case of dilute systems. This concept is discussed in detail in Mn impurities in Ni showing the clear difference of the spectra of the emitted photons when the excitation is at L_3 and about 4 eV above L_3 where transitions to lower spin states are important

(ii) the measurements as in the preceding case, but in the so-called forbidden (or perpendicular) geometry in which the incidence of the photons is normal to the magnetisation. In this case one considers a scattering channel bringing to a shallow core hole in the final state. In this case the absorption MCD is zero and the dichroism is seen only in the scattering. The process is able to detect the quadrupolar space distribution of the core hole coupled to the magnetic valence electrons. Results on Ni in Ni-ferrite and in Co metal are presented.

(iii) the experiments in the forbidden geometry with final shallow core hole in which one measures directly the integral of the emitted photon spectrum in the considered scattering channel. This integrated value is measured as a function of the incident energy and of the emission angle. The sum rules appropriate to this process are briefly discussed, showing how to recover ground state information which can hardly be obtained with other methods. Examples are given on Co-metal and on Co-ferrite.

The interest and the limitations of the methods are discussed and the perspectives are outlined.

e-mail: lucio.braicovich@fisi.polimi.it

Some Consequences of Relativistic Effects upon Optical Spectra

M.S.S. Brooks
European Commission, Joint Research Center, Institute for Transuranium Elements, D-76125 Karlsruhe, Germany

Abstract

Large spin-orbit interaction produces large orbital magnetic moments. Since the orbital character of the wave functions is more important in orbital than in spin magnetism, the limitations of the local spin density approximation become evident. It is possible to keep the orbital dependence of the exchange interactions by using Hatree-Fock theory with shielded Slater integrals for exchange while keeping most of the local density approximation for the charge density. Calculation of the full density matrix is involved - including that part off-diagonal in spin. This leads to an enhancement of the calculated orbital moment when the magnetism is strong. There is also a reduction in the calculated total spin moment and enhancement of non-collinear spin density (due to the off-diagonal spin density matrix) when the magnetism is weak. Recent calculated magnetic moments, form factors and dichroism spectra are decribed.

Soft x-ray resonant magnetic scattering from patterned magnetic materials

E. Dudzik[1], S. S. Dhesi[2], G. van der Laan[3],
[1] *Hahn-Meitner-Institut, Glienicker Str. 100, D-14109 Berlin*
[2] *ESRF, Grenoble, France,*
[3] *Daresbury Laboratory, Warrington Wa4 4AD, UK*
K. Chesnel[4], M. Belakhovsky[4], B. Gilles[4], S. Landis[4]
[4] *DRFMC, CEA Grenoble, France*

Abstract

Patterned materials and thin films with perpendicular magnetic anisotropy are currently of interest as promising materials for increasing data storage densities. These structures have dimensions of the order of magnitude of 10^2 Å, which make them well suited for diffraction studies with soft x-rays which have wavelengths around 15 Å. To enhance the magnetic scattering amplitude, the photon energy is tuned into an absorption edge.
We have studied magnetic lines and dots grown by depositing CoPt multilayers on patterned Si substrates, using resonant magnetic scattering, both with specular reflectivity and transverse scans. This method yields both structural and magnetic information, and gives evidence for antiferromagnetic coupling between neighbouring lines. This coupling depends on the spacing and the geometry of the substrate pattern, with a critical distance needed between dots to isolate them magnetically.
We have also studied a series of FePd thin films with perpendicular magnetic anisotropy. This anisotropy can be tailor-made by varying film growth conditions, and allows the stacking of layers of various anisotropies to produce different magnetic depth profiles in a single material. These profiles can be detected using resonant magnetic scattering.

Interface magnetic anisotropy in Fe/CeH_2 multilayers probed by the resonant diffraction of soft x-rays

H.A. Dürr[1)], M. Münzenberg[2)],
W. Felsch[2)], S.S. Dhesi[3)],
[1)] IFF, Forschungszentrum Jülich, Germany,
[2)] I. Phsikalisches Institut, Universität Göttingen, Germany,
[3)] ESRF, France.

Abstract

The interfaces between magnetic and non-magnetic layers often determine magnetic properties such as the magneto-crystalline anisotropy (MCA). At transition metal (TM) / rare earth (RE) interfaces the indirect exchange coupling between TM $3d$ and RE $4f$ shell mediated by the RE $5d$ electrons induces a significant $4f$ magnetic moment. In a single-ion anisotropy picture the strong crystalline field of the TM interface atoms acting on the large orbital quadrupole moment of the RE $4f$ shell is expected to pull the spins out-of-plane.

We used x-ray resonant magnetic scattering to corroborate this mechanism in Fe/CeH_2 multilayers. Interface sensitivity was achieved by setting up x-ray standing wave fields near the multilayer Bragg peaks. First and second-order magnetic scattering contributions were separated utilizing the magnetic domain structure of the sample. While the first-order contribution measures mainly the magnetic moment the second-order contribution is directly related to the MCA of the studied element. Temperature dependent measurements reveal that the single-ion anisotropy contributes to the total MCA only at temperatures far below the spin reorientation transition, T_R. Near T_R an MCA contribution dominates which is induced at the Fe interface atoms via electronic hybridization effects.

Transmission X-ray Microscopy using X-MCD

T. Eimüller
Univ. Würzburg, Experimentalphysik IV, AG. G. Schütz

Abstract

The X-ray Magnetic Circular Dichroism (X-MCD) can be used as a large, element-specific and quantitative magnetic contrast mechanism in Transmission X-ray Microscopy (TXM) [1,2]. The functionality and the potential of the novel method of Magnetic Transmission X-ray Microscopy (MTXM) will be outlined. The high spatial resolution of 30 nm and the possibility to image in varying external magnetic fields allowed to investigate the domain structure and the magnetization reversal of multilayered and laterally nanostructured FeGd systems. The switching behavior of a dot array was studied and a correlation between the nucleation field and the perimeter of each dot could be found. As the X-MCD contrast is directly proportional to the magnetization of the sample hysteresis loops of individual dots could be deduced. Recent results obtained with Fe films show that the method is not only restricted to perpendicular magnetized systems but can also used for technologically important in plane magnetized systems.

[1] P. Fischer, T. Eimüller, G. Schütz, P. Guttmann, G. Schmahl, K. Prügl und G. Bayreuther, *J. Phys. D: Appl. Physics* **31**(6), 649 (1998)
[2] T. Eimüller, R. Kalchgruber, P. Fischer, G. Schütz, P. Guttmann, G. Schmahl, M. Köhler, K. Prügl, M. Scholz, F. Bammes and G. Bayreuther, *J. Appl. Phys.* **87**, 6478 (2000)

Studies of magnetic x-ray spectroscopy from localized to itinerant materials

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

Abstract

An overview will be given of magnetic dichroism in x-ray absorption, photoemission and scattering covering 3d transition metals, rare earths and actinides. Theoretical models will

discussed and compared with recent experimental results. It is shown how the spectral structure of the magnetic circular dichroism (MCD) in core-level spectroscopy can be analysed using angular momentum algebra. The results are supported by full-multiplet calculations in intermediate coupling, which for localized materials are in very good agreement with the experimental results. On the other hand, for itinerant metals, such as nickel and iron, the 2p photoemission spectra do not agree with a one-particle model. Recent experimental results for the Ni 2p photoemission of nickel metal show that inter-configurational mixing has to be taken into account in order to understand the detailed structure of the MCD. Apart from its invaluable use to quantify the ground-state spin and orbital magnetic moments, MCD therefore also provides a powerful tool to study, in an element-specific way, the electron-correlation effects arising in a large variety of materials. Of special interest are thin films, where the transition from localized to itinerant and its influence on the magnetic properties, can be monitored as a function of the film thickness.

Soft x-ray magnetic diffraction with coherent beams: towards magnetic speckle spectroscopy

Jeroen Goedkoop
Condensed Matter Physics, Van der Waals Zeeman Institute
University of Amsterdam

Abstract

Traditionally, x-ray diffraction was a matter of hard x-rays. Currently, this situation is changing by the growing awareness that the spectroscopic information contained in soft x-ray edges can be exploited in anomalous scattering experiments to obtain electronic or magnetic information on nanometer length scales. Thus, it has recently become possible to study the magnetic domain structures in thin films and surfaces using soft x-ray magnetic scattering experiments. With the present flux and detectors, soft x-ray diffraction experiments can resolve magnetic domain structures with a resolution of 30 nm. A unique feature of this technique compared to microscopic techniques is the possibility to obtain 3 dimensional information.

The next step in this development is the exploitation of the coherence available at third generation sources. In this talk we will demonstrate the possibility to obtain sufficient coherent flux to obtain magnetic x-ray speckle patterns from static magnetic domain structures in thin films. Possible applications of speckle spectroscopy for the study of magnetic fluctuations will be discussed.

X-ray Magneto-Optics in Lanthanides

F. Heigl, A. Vollmer, G. Kaindl, and K. Starke
Institut für Experimentalphysik, Freie Universität Berlin,
Arnimallee 14, D–14195 Berlin-Dahlem, Germany

Abstract

Magneto-optical methods in the visible light regime generally lack element-specificity, which has become a considerable shortcoming in research on advanced heteromagnetic systems. Using circularly polarized soft x rays tuned to a 4d-4f core-level transition of a lanthanide element, the specularly reflected x-ray intensity changes proportionally to the magnetization of this element and, e.g. hystereses are easily measured element-specifically. In contrast to using visible light, temperature de-pendent 4d-4f magneto-optical signals are not influenced by the thermal lattice expansion.
This work is supported by BMBF (05 SC6 KEB-8) and the DFG (Sfb 290).

Electronic Ordering and Excitations in Transition Metal Oxides

John Hill
Brookhaven National Lab, Physics Department
Upton, NY 11973-5000

Abstract

The physics of the transition metal oxides is dominated by the strongly correlated electron behavior, which results in the large diversity of electronic ground states. Understanding the electronic ordering and excitations of these ground states is thus critical to understanding these materials. Here, we discuss x-ray scattering studies of electronic ordering - specifically charge and orbital ordering - in the manganites, and electronic excitations in the cuprates. Studies of the charge and orbital order parameters are presented in a number of manganites. At very high temperatures, we observe weakly correlated orbital fluctuations that appear common to manganites with dissimilar ground states. At low temperatures, in insulating samples, a charge and orbitally ordered state is observed with long range charge correlations and short range orbital correlations. Pretransitional fluctuations in such samples suggest that the charge ordering drives this phase transition. The studies of electronic excitations focused on a one dimensional cuprate, $CuGeO_3$, and utilized resonant inelastic x-ray scattering at the Cu K-edge. Three excitations were observed, a charge transfer excitation, an exciton-like excitation and an orbital, or d-d, excitation. The last two are localized excitations and exhibit no dispersion. However, the charge transfer excitation disperses along the chain direction and appears to be sensitive to the spin-spin correlation function.

Element-selective mapping of spin and orbital moments by magnetic circular dichroism microspectroscopy

W. Kuch, and J. Kirschner
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2,
D-06120 Halle, Germany

Abstract

The combination of x-ray magnetic circular dichroism (XMCD) in soft x-ray absorption and photoelectron emission microscopy (PEEM) can be used to obtain locally resolved magnetic information on a microscopic scale. Scanning the photon energy across elemental absorption edges and recording microscopic images of the local secondary electron intensity for both photon helicities at each photon energy step allows to analyze local XMCD spectra at any position of the imaged area of the sample. Applying sum rules, local quantitative information about spin and orbital magnetic moments can be extracted from such microspectroscopic measurements. The full power of XMCD as spectroscopic tool is so maintained; in addition, microscopic spatial resolution is added.
This approach is used to study spin reorientation transitions in magnetic ultrathin bilayer films. Co/Ni/Cu(001) epitaxial films exhibit a spin reorientation transition of the magnetic easy axis from perpendicular to the film plane to in-plane as a function of both Co and Ni film thicknesses. Images of the Ni spin magnetic moment composed of 76800 single-pixel local absorption spectra of 370×370 nm^2 size reveal the absolute value of the spin moment and the magnetic domain structure. The ratio of orbital to spin moment yields information about element-resolved local magnetocrystalline anisotropy. In the case of Co/Ni/Cu(001), the Ni orbital to spin moment ratio shows distinctly higher values for out-of-plane magnetization than for in-plane magnetization. From this an out-of-plane magnetocrystalline anisotropy of the Ni film can be deduced.

Exploring the microscopic origin of exchange bias with Spectromicroscopy

A. Scholl[1], F. Nolting[12], H. Ohldag[123], J. Stöhr[2], J. Lüning[2], S. Anders[4], H.A. Padmore[1]

[1]Advanced Light Source, 1 Cyclotron Road, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

[2]Stanford Synchrotron Radiation Laboratory, P.O. Box 20450, Stanford, CA 94309, USA

[3]Universität Düsseldorf, Institut für Angewandte Physik, Universitätsstraße 1, 40225 Düsseldorf

[4]IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, CA 95120, USA

Abstract

Despite large experimental and theoretical efforts the origin of exchange bias at the interface of ferromagnets and antiferromagnets is still controversial, mainly because detection of the interfacial magnetic structure is difficult. We have applied photoelectron emission microscopy on several ferromagnet - antiferromagnet thin-film structures and microscopically imaged the ferromagnetic and the antiferromagnetic structure with high spatial resolution. Taking advantage of the surface sensitivity and elemental specificity of PEEM the magnetic configuration and critical properties such as the Neel temperature were determined on LaFeO3 and NiO thin films and single crystals. On samples coated with a ferromagnetic layer we microscopically observe exchange coupling across the interface, causing a clear correspondence of the domain structures in the adjacent ferromagnet and antiferromagnet. We

can even observe the domain structure due to uncompensated magnetic moments in the antiferromagnet which is found to completely match that of the ferromagnet. Field dependent measurements reveal a strong uniaxial anisotropy in individual ferromagnetic domains and a local exchange bias even in not explicitly field-annealed samples, caused by interfacial uncompensated magnetic spins. We have measured remanent hysteresis loops in sub-micrometer domains as function of domain size showing bias fields of up to 30 Oe in Co / LaFeO3. These experiments provide highly desired information on the relative orientation of electron spins at the interface between ferromagnets and antiferromagnets, which is of key interest for an eventual understanding of the exchange bias phenomenon.
This work was supported by the Director, Office of Basic Energy Sciences, of the US Department of Energy.

Ab-Initio Theory of MXRS and DAFS

E. Arola and P. Strange
Theoretical Physics Group, School of Chemistry and Physics, Keele University, Keele, Staffordshire, ST5 5BG.

Abstract

We present a description of a first principles formalism for the scattering of circularly polarized x-rays within the framework of relativistic density functional theory (DFT). The scattering amplitudes are calculated using standard time-dependent perturbation theory to second order in the electron-photon interaction vertex. Two implementations of the theory are discussed, one based on relativistic spin-polarized multiple scattering theory, and a second based on relativistic Self-Interaction Corrected DFT and the LMTO method. The former method is easier to implement, but the latter makes the theory applicable to rare earth materials where many MXRS experiments have been performed. The theories will be illustrated with appropriate examples.

Magnetic circular dichroism in x-ray absorption: MEXAFS and XMCD

H. Wende, F. Wilhelm, P. Poulopoulos, A. Scherz, and K. Baberschke
Institut für Experimentalphysik, Freie Universität Berlin,
Arnimallee 14, D–14195 Berlin-Dahlem, Germany

Abstract

In order to demonstrate the large potential of the X-ray absorption spectroscopy in the extended- and the near-edge regime we will present three experiments which allow for new insights into magnetism.

i) First we will discuss the magnetic EXAFS (MEXAFS) at the L-edges of a Gd single crystal, i.e. in an extended photon-energy range of 7100-8500 eV. As the EXAFS technique, MEXAFS provides information in real-space on a nearest-neighbor scale. Therefore the effect of dynamic disorder on the spin-pair distribution function can be analyzed by means of

temperature-dependent MEXAFS investigations. On the other hand the near-edge XMCD is recorded in the same spectra and probes the long-range magnetic order, i.e. the magnetization of the sample. Furthermore the spin-dependent scattering of the photoelectron which is responsible for the MEXAFS, leads to an enhancement of the multiple-scattering contributions compared to the spin-averaged EXAFS [1].

ii) As an example for the application of the near-edge XMCD technique we will present results for Ni_n/Pt_m multilayers. Measuring the XMCD at the Ni and Pt $L_{3,2}$-edges we were able to construct a layer-resolved magnetic moment profile for a Ni_6/Pt_5 multilayer for **both** elements. These results are compared to *ab initio* tight-binding LMTO calculations. It turns out that Pt is a strongly polarizable magnet [2].

iii) For the same Ni/Pt multilayers we carried out angular dependent XMCD measurements. This allowed us to determine the anisotropy of the orbital moment μ_L. The careful analysis revealed possible pitfalls for the determination, e.g. saturation effects must be corrected. As hysteresis loops have been measured for the samples by means of a vibrating sample magnetometer the relation of the magnetic anisotropy energy can be related to the difference of the orbital moments $\Delta\mu_L = \mu_L^{\perp} - \mu_L^{\parallel}$ [3].

This work is supported by BMBF (05 SC8 KEA-3), the DFG (Sfb 290) and ESRF (HE-422).

[1] H. Wende *et al.*, AIP Conference Proceedings **514** (2000) 140.
[2] F. Wilhelm *et al.*, Phys. Rev. Lett. **85** (2000) 413.
[3] F. Wilhelm *et al.*, Phys. Rev. B, **61** (2000) 8647.

Abstracts of poster contributions:

A relativistic description for the magnetic Compton scattering of solids

D. Benea and H. Ebert
Department Chemie / Physikalische Chemie, Universität München,
Butenandstr. 5-13, D-81377 München, Germany

Abstract

A fully relativistic calculation of spin resolved density of momentum is presented and a scheme to determine the magnetic Compton profiles for magnetic solids. This formalism is set up within the framework of spin-polarised relativistic Koringa-Kohn-Rostoker (SPR-KKR) method of bandstructure calculations. This 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 authors and experimental data. Also the effects of disorder on the momentum density are studied and the corresponding computed Compton profiles for ordered and disordered alloys are presented.

Magneto-optical properties of multilayer- and surface layer systems

Tilman Huhne, Alexander Perlov and Hubert Ebert
Inst. für Physik. Chemie, Universität München,
Butenandtstr. 5-13,81377 München
Germany

Abstract

Magneto-optical spectra of magnetic solids in the visible regime provide a lot of information which enable one a deep insight into the electronic structure. While the corresponding experimental measurements are relatively easy to carry out, the interpretation of the spectra is quite complicated because of the interference of the effects of many electronic transitions involved. For this reason, the theoretical calculation of magneto-optical effects on the basis of ab-initio bandstructure calculations is an important means for the decoding of the experimental data.

Our method for the calculation of the frequency dependent, layer resolved optical conductivity for multilayer and surface layer systems, which has been presented earlier, allows to deduce all experimentally observable magneto-optical quantities. It is based on the self-consistent ab-initio Green's function method (KKR-GF).

The program has been extended for the use of the Tight-Binding KKR-method which enables us to treat more realistic, larger layer systems of up to 30 perturbed layers.

We present results for bulk Fe, Co, and Ni, as well as Au/Fe and Cu/Co surface layer systems which are, as far as possible, compared with the results of other authors and the experiment.

Transverse Magneto-optical Kerr-effect and angle resolved photoemission from 3d metals on W(110)

V. Senz, A. Kleibert, K.H. Meiwes-Broer, and J. Bansmann

Abstract

Tunable linearly and circularly soft X-ray radiation opens the possibility for a couple of powerful methods in investigating magnetic properties of thin films, islands, and nanoparticles on surfaces, such as magnetic dichroism in angle resolved photoemission (MDAD), X-ray magnetic circular dichroism in photoemission (XMCD) and in-situ Magneto-optics at the core levels (MOKE).

Here, we will present new data from recent measurements using the transverse MOKE (T-MOKE) at iron films and islands on W(110). The measurements themselves have been carried out at the U49/1 SGM undulator beamline at BESSY II using linearly polarized radiation. For recording hysteresis curves we have applied an external electromagnet (B<0.5T)

to the experimental setup. Close to the Fe 2p core levels the reflectivity and the Kerr rotation is strongly enhanced by resonant forward scattering. We could observe huge intensities in reflexion and, moreover, intensity differences up to 50% at iron films of only 5ML. When annealing epitaxially grown Fe(110) films on W(110) above 500°C a well oriented Fe island structure can be created (easily visible in LEED). We have analyzed the rotation of the easy magnetization axis of such self-organized islands with respect to the behavior of epitaxial iron films. Our experimental data clearly show a rotation of the easy axis which depends on the original coverage of the iron films before annealing. A rotation of the easy magnetization axis was already detected in earlier MDAD photoemission experiments [1] but at that time only measurements in remanence were possible.

1

L. Lu, J. Bansmann, K.H. Meiwes-Broer, J. Phys. Cond. Matter 10 (1998) 2873

Spin-resolved NEXAFS from resonant X-ray scattering (RXS)

Guenter Draeger*, Thomas Kirchner*,
Sergej Bocharov*, Chi-Chang Kao**
* Fachbereich Physik, Universitaet Halle, 06108 Halle, Germany
** NSLS, Brookhaven National Laboratory,
Upton, New York 11973 USA

Abstract

Resonantly excited metal K and L core line spectra of MnO, Fe2O3, NiO, CuO and Dy3Fe5O12 have been investigated at the beamlines X21 (NSLS/BNL), W1.1 and BW1 (HASYLAB/DESY). From analysis of spectral data the following conclusions can be drawn: - spin conservation is valid in the scattering process, for excitations below the absorption threshold as well as above it, - the absorption thresholds are different for spin-up and spin-down components of resonantly scattered spectra, - quadrupole transitions are very important or even crucial in the excitation process. With this experience a novel technique for quantitative resolution of NEXAFS spectra into spin-up and spin-down components has been developed. Since the method employs spin conservation and local spin references, it needs no circularly polarized radiation and no sample magnetization for taking both the RXS and NEXAFS spectra. Hence antiferromagnetic and paramagnetic materials can be investigated as well. Utilizing linear dichroism by angular-dependent measurements at single-crystal samples additional resolution of NEXAFS spectra is possible with respect to the orbital symmetry. Application of the method to single-crystal antiferromagnetic NiO and paramagnetic MnO, for the first time, provides new and unambiguous experimental results confirming modern (LSDA+U) calculations: The metal K pre-edge XAS of NiO and MnO has predominantly 3d(eg) spin-down and 3d(t2g and eg) spin-down character, respectively. On the other hand, the delocalized p-like states, arising from the p-d band effect hybridization have spin-up character.

Resonant Magnetic X-Ray Scattering in the Hard and the Soft X-Ray Region: Magnetic Structure of Lanthanide Films

C. Schüßler-Langeheine, E. Weschke, H. Ott,
A.Yu. Grigoriev,R. Meier, D.V. Vyalikh,
Chandan Mazumdar, and G. Kaindl
Institut für Experimentalphysik, Freie Universität Berlin,
Arnimallee 14, D-14195 Berlin-Dahlem, Germany
C. Sutter, D. Abernathy, and G. Grübel
European Synchrotron Radiation Facility,
B.P. 220, 38043 Grenoble-Cedex, France

Abstract

The temperature-dependent magnetic structures of epitaxial Ho and Dy metal films were studied by resonant magnetic x-ray scattering, using photon energies corresponding to the L3 and M5 absorption edges. In both cases, the experiments were carried out in special ultrahigh-vacuum setups, with the films being prepared *in situ* on W(110). They reveal high crystalline quality with mosaic spreads of $\approx 0.04°$.
Hard x-ray studies show that a Ho film with a thickness of $\approx$ 110 monolayers exhibits a bulk-like magnetic structure in the helical antiferromagnetic phase. The ferromagnetic-antiferromagnetic phase transition in a 180-monolayer-thick Dy film, however, displays an anomalous hysteresis of the magnetic-satellite intensity, indicating clamping of the ferromagnetic phase and temperature-dependent growth of antiferromagnetic domains up to 30 K above the Curie temperature.
While these investigations at the L3 edges, although taking advantage of the resonant enhancement of the magnetic scattering cross section by a factor of $\approx$ 50, are limited to films with thicknesses larger than $\approx$ 30 monolayers, the huge resonant enhancement at the M5 edges of the lanthanides allows to extend the studies to films with thicknesses of 10 monolayers or even less. This is demonstrated for the case of Ho metal, revealing that the enhancement of the magnetic scattering cross section is of the order of 10^6. It is found that the magnetic period of bulk Ho metal in the antiferromagnetic phase essentially persists down to 15 monolayers, while it has substantially changed at 10 monolayers, i.e., for comparable magnitudes of magnetic period and film thickness.

XMCD at $L_{II,III}$ edges of Rare-Earths: quadrupolar and dipolar effects

Ch. Giorgetti, E. Dartyge, F. Baudelet *, Ch. Brouder **

Abstract

X-ray Magnetic Circular Dichroism at $L_{II,III}$ edges of Rare Earths in Rare Earth-3d Transition Metal compounds is still a subject of study, specially the separation between E1

and E2 contributions. E2 transitions can be evidenced by studying the XMCD spectra as a function of the angle θ between the quantization axis of the compound and the wave vector of incident photons. The XMCD(E2) of a powder is proportional to

[s1 cos θ + s 3 (3 − 5 cos^2 θ)/2], where s1 and s3 are the spherical tensors of order 1 and 3 [1] since the XMCD(E1) is proportional to cos θ. Then any deviation to cos θ dependence sign the presence of E2 transitions. We will present experimental evidence of quadrupolar electric transitions at L_{III} *and* L_{II} edges of Er in $ErFe_2$ Laves phase. These results will be compared with atomic calculation taking into account crystal electric field effects on Er site.

[1]. Ch. Brouder, Compte-rendu des Journées Grand-Est, Strasbourg 6-7 Janvier 1994

Metal-to-insulator transition in Rare-Earth hydride /Fe multilayers: Interface polarization measured with XMCD

M. Münzenberg [1], F. Leuenberger[1], T. Neisius[3], S. Pizzini [2], W. Felsch[1], N.A. Fontaine[2], and S. Pascarelli[3],

[1]I. Physikalisches Institut and SFB 345, Bunsenstr. 9, 37073 Göttingen, Germany
[2]Lab. Louis Néel, CNRS, BP 166, 38042 Grenoble Cedex, France
[3]ESRF, BP 220, 38043 Grenoble Cedex, France

Abstract

In REH_x/Fe multilayers (RE=Ce, La, Gd) the electronic properties of the RE-hydride interlayers may be switched between metallic and insulating by varying the hydrogen content x. For a systematic investigation, multilayers with different REH_x-thicknesses were prepared. Measurements of X-ray absorption and X-ray magnetic circular dichroism (XMCD) at the L_2 and L_3-edges of the RE show the change in the electronic structure of the empty 5d-electron states across the metal-to-insulator transition: The white line increases and the magnetic polarization at the interfaces induced by Fe via 3d-5d hybridisation decreases by a factor of two, but does not vanish. This can be studied gradually at the transition. The line shape of the XMCD signal shows a characteristic modification. It is discussed in a model employing two parameters, which represent a shift in energy and (in the case of Ce and Gd) a difference in the 2p →5d dipole matrix element for the two spin states of the excited photoelectron [M. van Veenendaal *et al.*, Phys. Rev. Lett. **78**, 1162 (1997); H. Matsuyama *et al.*, J. Phys. Soc. Jpn. **66**, 337 (1997)].

X-Ray Faraday Effect at the $L_{2,3}$-Edges of Fe, Co, and Ni: Experiment and Theory

H.-Ch. Mertins, F. Schäfers, A. Gaupp, and W. Gudat
BESSY GmbH, Albert-Einstein-Str. 15, D-12489 Berlin, Germany
J. Kuneš and P. M. Oppeneer
Institute of Solid State and Materials Research,
P.O. Box 270016, D-01171 Dresden, Germany

Abstract

The X-ray Faraday effect at the $L_{2,3}$ edges of the $3d$ ferromagnets Fe, Co, and Ni is studied both experimentally and theoretically. Experimental spectra are measured with linearly polarized soft-X-ray synchrotron radiation at BESSY, Berlin. Our measured X-ray Faraday rotations are remarkably large, up to 2×10^5 degree/mm, which is more than one order of magnitude larger than those observed in the visible. At a grazing angle of incidence the Faraday rotations of films of 100–300 nm thickness can reach values of $\pm 90°$. The measured X-ray Faraday rotation and ellipticity spectra are compared to theoretical spectra which we calculated within the framework of the local spin-density approximation and that of the Kubo linear-response formalism. Our calculated Faraday rotation and ellipticity spectra are in good quantitative correspondence with the measured spectra. We deduce from the measured spectra the dichroism $\Delta\delta$, $\Delta\beta$, in the dispersive, absorptive part, respectively, of the index of refraction, $n^{\pm} = 1 - (\delta_0 \pm \Delta\delta) + i(\beta_0 \pm \Delta\beta)$, and compare these to *ab initio* calculated dichroic refractive indices. The satisfying quantitative agreement of experimental and theoretical dichroic spectra illustrates that a single-particle approach, based on the local spin-density functional theory, may provide an accurate description of magneto-X-ray effects.

(For the complet list see: http://www.physik.fu-berlin.de/ starke/xrms2000)

3.2 Reports on Visits to Conferences/Workshops

Report on a Conference Participation:

The 8th Joint MMM-Intermag Conference

San Antonio, Texas

January 7-11, 2001

The Joint MMM-Intermag Conference was attended by about 4000 people from Europe, Japan, Latin America and the USA. The conference was very exciting and gave a representative overview of the activities in the field of magnetism including basic research and applications. In a lively atmosphere the participants were able to exchange new scientific results.

I can not present a general overview of the conference since the meeting was organized in more than 20 parallel sessions per day. Highly interesting topics were magnetic tunnel junctions, spin injections in semiconductors and oxides, exchange bias, manganites and manganite thin films, spin-transport in nanotubes, patterned media and many more.

Very interesting was the symposium on spin transport. Invited talks were presented by J.C. Lodder (Enschede) on the hot-electron spin-transport, by J. Byers (Washington) on theory of spin injection, by R. Buhrman (Ithaca), on spin-transfer excitation and switching in thin film nanomagnets, by H. Ohno (Sendai) on spin-injection in ferromagnetic semiconductors, by T. Dietl (Warszawa) on theory of ferromagnetic interaction in doped semiconductors, and by L. Molenkamp (Würzburg) on dilute magnetic semiconductors in spin-polarized electronics.

Activities of the TMR network "Interface Magnetism" were also presented: one contribution on "Microscopic origin of giant magnetoresistance" (Dresden) and another on "Theory of tunneling magnetoresistance" (Dresden).

Ingrid Mertig

4 News from the Research Training Network (RTN)

COMPUTATIONAL MAGNETOELECTRONICS

4.1 Workshop/Conference Announcements

4.1.1 First Annual Meeting

First Announcement

1st Annual Meeting
of the Research Training Network
Computational Magnetoelectronics

Budapest, September 27-30, 2001

organized by the Hungarian Partner

Objective: The purpose of the meeting is to provide an overview on the activity of all the partners of the Network during the first year, Oct 2000 – Sept 2001. On average 5–10 members per each node (in total up to 80 participants) are expected, with special attention to young researchers for whom a session of tutorial lectures given by senior researchers is scheduled. We also plan to invite a limited number of overseas participants (non-members of the Network). All participants are invited to give oral contributions covering the topics of the scientific projects of the Network. Plans on research and training collaborations within the Network, on future workshops and realization of the scientific programs will be extensively discussed.

Timetable:	Sept 27, Thu Morning	Arrival
	Sept 27, Thu 2 p.m. – Sept 30, Sun 12 a.m.,	Meeting
	Sept 30, Sun Afternoon	Departure

Venue: The meeting will be held in the conference room of Hotel *AGRO, H-1121 Budapest, Normafa u. 54*, which is located at the attractive, hilly side of Budapest. Accommodation will be provided in single and double rooms in the same hotel or nearby.

Attendance: In order to get a quick overview on how many people are expected, we ask the node leaders (spokespersons) for sending us a list of the scheduled participants from the corresponding node. Please, also make notes on the list about the need for single and double

rooms (and the tentative sharing). Please, also mark on the list the tentative time of arrival and departure of the participants.

Further details and the scheduled program will be announced in the forthcoming Newsletters. The abstracts of the contributions will be collected into an abstract booklet which will be distributed prior the meeting.

Contact: János Kollár `jk@szfki.hu`
László Szunyogh `szunyogh@heisenberg.phy.bme.hu`

4.2.1 Report on GMR/TMR Workshop

Research Training Network (RTN)
on Computational Magnetoelectronics

Workshop on TMR and GMR

Dresden, December 01 - December 03, 2000

supported by:

RT-Network on "Computational Magnetoelectronics"

Max-Planck-Institut für Physik komplexer Systeme

SFB 422 – "Strukturbildung und Eigenschaften in Grenzschichten"

The workshop was held at the Max Planck Institute for the Physics of Complex Systems in Dresden, on the weekend of December 01-03, 2000. It was organized by Ingrid Mertig and was sponsored by the RT-Network on Computational Magnetoelectronics, the Max Planck Institute for the Physics of Complex Systems in Dresden, and the Sonderforschungsbereich 422, TU Dresden. The workshop was attended by 54 participants.

As the enclosed program and abstracts indicate, we covered the area of Tunneling Magnetoresistance (TMR), Giant Magnetoresistance (GMR), Andreev reflection, current-induced coupling and switching in layered magnetic structures. Ab initio calculations of these properties were in the center of interest. These talks have been nicely completed by talks on new experiments in the field and by talks on phenomenological models (J. Barnas, Poznan, C.Lambert, Lancaster, A. Vedyayev, Moscow).

One of the most interesting TMR systems is Fe/MgO/Fe. The system is grown epitaxially and allows a comparison of theory and experiment. A number of very interesting talks were dedicated to this topic. A. Fert (Paris) and W. Wulfhekel (Halle) presented very new experimental results. Different theoretical approaches were presented by J. Mathon (London), M. Freyss and D. Wortmann (Jülich), M. Zwierzycki (Twente), J. Henk (Halle) and P. Zahn (Dresden). The problem of hot spots in the ab initio calculations for electron tunneling was successfully attacked by V. Drchal (Prague) and O. Wunnicke (Juelich). Highly sophisticated results of tunneling through the more complex alumina barrier were discussed by E. Tsymbal (Oxford) and semiconducting barriers have been investigated by A. Perlov (München) and P. Weinberger (Wien).

The ab intio calculations of GMR are already much more refined than the TMR calculations. Different methods are used to investigate GMR. The calculations are either based on Kubo's (C. Blaas, Wien) or Landauer's formula (J. Kudrnovsky, Prague, and K. Xia, Twente) or start from the Boltzmann equation (J. Binder, Dresden). The calculations offer a very good insight into the microscopic origin of GMR and can even reproduce experimental trends.

A. Fert (Paris), P. Levy and C. Heide (New York) presented an interesting overview about current-induced coupling and switching.

New questions like spin injection (G. Schmidt, Würzburg) and Andreev reflection (W. Belzig, Delft) or systems of potential interest in microelectronics Ca B_6 (P. Kelly, Twente) and Manganites (van den Brink, Twente) were addressed. A. Lichtenstein (Nijmegen) and A. Ernst (Halle) discussed the influence and the treatment of correlation effects.

In total, it was a scientifically interesting meeting with many lively discussions.

Ingrid Mertig

List of Participants

Nr.	Name	e-mail
1.	Abrikosov, Igor	Igor.Abrikosov@fysik.uu.se
2.	Annett, James	james.annett@bristol.ac.uk
3.	Barnas, Jozef	barnas@spin.amu.edu.pl
4.	Bauer, Gerrit	g.e.w.bauer@tn.tudelft.nl
5.	Belzig, Wolfgang	W.Belzig@tn.tudelft.nl
6.	Binder, Jörg	J.Binder@physik.tu-dresden.de
7.	Blaas, Claudia	cb@cms.tuwien.ac.at
8.	Bruno, Patrick	bruno@mpi-halle.de
9.	Chshiev, Mairbek	chshiev@ipcms.u-strasbourg.fr
10.	Dederichs, Peter	l.gerken@fz-juelich.de
11.	Drchal, Vaclav	drchal@fzu.cz
12.	Ebert, Hubert	he@gaia.cup.uni-muenchen.de
13.	Ernst, Arthur	aernst@mpi-halle.de
14.	Fert, Albert	fert@lps.u-psud.fr
15.	Freyss, Michael	M.Freyss@fz-juelich.de
16.	Henk, Jürgen	henk@mpi-halle.de
17.	Herper, Heike	heike@thp.uni-duisburg.de
18.	Holstrom, Erik	Erik.Holstrom@bristol.ac.uk
19.	Hong, J.	jhong@mpi-halle.de
20.	Kelly, Paul	p.j.kelly@tn.utwente.nl
21.	Kosuth, M.	km@eeb03.cup.uni-muenchen.de
22.	Kudrnovsky, Josef	kudrnov@fzu.cz
23.	Lambert, Colin	c.lambert@lancaster.ac.uk
24.	Levy, Peter	levy@nyu.edu
25.	Lichtenstein, Alexander	A.Lichtenstein@sci.kun.nl
26.	Mathon, George	J.Mathon@city.ac.uk
27.	Mertig, Ingrid	mertig@theory.phy.tu-dresden.de
28.	Mirbt, Susanne	susanne@fysik.uu.se
29.	Newman, C.	
30.	Opitz, Jörg	opitz@theory.phy.tu-dresden.de
31.	Papanikolaou, Nikos	N.Papanikolaou@fz-juelich.de
32.	Pattison, N.	
33.	Perlov, A.	ap@eeb09.cup.uni-muenchen.de
34.	Popescu, V.	vp@thetis.cup.uni-muenchen.de
35.	Riedel, Ingmar	ingmar@ptprs1.phy.tu-dresden.de
36.	Ryzhanova, Natalya	vedyayev@ipcms.u-strasbourg.fr
37.	Schmidt, Georg	georg.schmidt@physik.uni-wuerzburg.de
38.	Sommers, Chuck	sommers@lps.u-psud.fr
39.	Szunyogh, Laszlo	szunyogh@heisenberg.phy.bme.hu

40.	Temmerman, Walter	W.M.Temmerman@dl.ac.uk
41.	Tsymbal, Evgueni	evgueni.tsymbal@materials.oxford.ac.uk
42.	van den Brink, Jeroen	jvdb@tn.utwente.nl
43.	Vedyaev, Anatoly	vedyayev@ipcms.u-strasbourg.fr
44.	Weinberger, Peter	pw@cms.tuwien.ac.at
45.	Wortmann, Daniel	D.Wortmann@fz-juelich.de
46.	Wulfhekel, Wulf	wulf@mpi-halle.de
47.	Wunnicke, Olaf	O.Wunnicke@fz-juelich.de
48.	Xia, Ke	xia@tn.utwente.nl
49.	Yavorsky, Bogdan	bogdan@theory.phy.tu-dresden.de
50.	Zahn, Peter	peter@theory.phy.tu-dresden.de
51.	Zavalicke, F.	florin@mpi-halle.de
52.	Zeller, Rudolf	ru.zeller@fz-juelich.de
53.	Zhuravlev, M.	zhur@Physik.Uni-Bielefeld.de
54.	Zwierzycki, Michael	M.Zwiezycki@tn.utwente.nl

Program

Friday, December 01, 2000

9:00-9:05	**Opening**
Chair:	**P.H. Dederichs,** Jülich
9:05-9:35	**W. Wulfhekel**, Halle Characterisation of crystalline Fe/MgO/Fe tunneling junctions by local tunneling
9:35-10:05	**J. Mathon**, London Theory of tunneling Magnetoresistance of Fe/MgO/Fe and Co/Cu/Vacuum/Co junctions
10:05-10:35	**M. Freyss**, Jülich Electronic structure and transport properties of tunnel junctions
10:35-11:00	**Coffee**
Chair:	**P. Kelly**, Twente
11:00-11:20	**P. Zahn**, Dresden Tunneling in Fe/MgO/Fe
11:20-11:40	**D. Wortmann**, Jülich Ab initio calculations of tunneling through MgO barriers on Fe(001)
11:40-12:10	**H. Ebert**, München Magneto-optical properties of multiplayer- and surface layer systems
12:10-12:25	**I. Riedel**, Dresden Transmission coefficients - a new formalism

12:25-14:00 **Lunch**

Chair: **G.E.W. Bauer**, Delft

14:00-14:45 **G. Schmidt**, Würzburg
Spin injection

14:45-15:15 **W. Belzig**, Delft
Spin accumulation and Andreev reflection in ferromagnetics wires

15:15-15:45 **A. Vedyayev**, Grenoble
Giant magnetoresistance in hybrid superconductor/ferromagnetic sandwich heterostructures

15:45-16:00 **C. Newman**, Lancaster
A study of conductance oscillations in mesoscopic Andreev interferometers in the presence of spin orbit coupling

16:00-16:30 **Coffee**

Chair: **P. Bruno**, Halle

16:30-17:00 **A. Lichtenstein**, Nijmegen
Correlation effects on spin-polarization in transition metals

17:00-17:30 **A. Ernst**, Halle
Ab initio electronic structure study of materials used in the TMR

17:30-17:50 **P. Kelly**, Twente
Quasiparticle calculations for CaB_6

17:50-18:20 **J. van den Brink**, Twente
A review of theoretical approaches to CMR in Manganites

18:20-19:30 **Dinner**

Chair: **P.H. Dederichs**, Jülich

19:30 Discussion (new network projects)

Saturday, December 02, 2000

Chair: **P. Levy**, New York

9:00-9:45 **A. Fert**, Paris
Experimental results on spin polarized tunneling and questions

9:45-10:15 **J. Barnas**, Poznan
Charge and spin degrees of freedom in ferromagnetic single-electron transistors

10:15-10:30 **M. Chshiev**, Strasbourg
Giant asymmetry of current and of tunnel magnetoresistance
in double barrier junctions

10:30-11:00 **Coffee break**

Chair: **J. Mathon**, London

11:00-11:15 **K. Xia**, Twente
Parameter-free calculations of spin-dependent transport

11:15-11:30 **M. Zwierzycki**, Twente
Ab initio calculations of tunneling magnetoresistance

11:30-11:50 **J. Henk**, Halle
Spin-dependent electron tunnelling through planar junctions revisited

11:50-12:20 **V. Drchal**, Prag
Hot spots in tunnelling magnetoresistance

12:20-12:40 **O. Wunnicke**, Jülich
Effects of interface states on tunnelling: A simple model

12:40-14:00 **Lunch**

Chair: **E. Tsymbal**, Oxford

14:00-14:30 **J. Kudrnovsky**, Prag
Topics in CPP-transport in multilayers

14:30-14:50 **J. Binder**, Dresden
GMR in Co/Cu and Fe/Cr multilayers – a comparison

14:50-15:20 **C. Lambert**, Lancaster
Enhancement of GMR due to spin mixing in magnetic multilayers
with superconducting contacts

15:20-15:50 **C. Blaas**, Wien
Electrical transport properties of bulk Ni_cFe_{1-c} alloys and
related spin-valve systems

15:50-16:05 **B. Yavorsky**, Dresden
Giant Magnetoresistance due to a domain wall in Fe: Ab initio study

16:05-16:30 **Coffee**

Chair: **S. Mirbt**, Uppsala

16:30-17:00 **P. Levy**, New York
Current-induced coupling

17:00-17:20 **C. Heide**, New York
Current-induced switching

17:20-17:40 **A. Fert**, Paris

	Experiments of magnetization reversal by spin injection
17:40-18:00	**N. Pattison**, Lancaster Current-induced torques in ferromagnetic nanostructures
20:00	**Dinner**
	Restaurant "Italienisches Dörfchen" Theaterplatz 3 (near Semper Opera)

Sunday, December 03, 2000

Chair:	**J. Kudrnovsky**, Prag
9:00-9:30	**E. Tsymbal**, Oxford Electronic structure of Co-Alumina tunnel junctions
9:30-10:00	**P. Weinberger**, Wien Perpendicular transport in Fe/Ge heterostructures
10:00-10:20	**D. Wortmann**, Jülich Resolving complex atomic-scale spin-structures by SP-STM
10:20-10:40	**I. Abrikosov**, Uppsala Magnetic properties of Co/Cu/Ni trilayer on the Cu(100) surface
10:40-11:10	**Coffee**
Chair:	**P. Weinberger**, Wien
11:10-11:30	**A. Perlov**, München Electronic and magnetic properties of ferromagnet-semiconductor heterostructure systems
11:30-11:50	**M.Ye. Zhuravlev**, Bielefeld The theory of GMR and TMR in segmented magnetic nanowires with surface roughness
11:50-12:10	**E. Holstrom**, Bristol Fermi surface flattening effects on magnetic interlayer coupling
12:10	**Closing remarks**
12:20	**Lunch**

Abstracts

Characterisation of crystalline Fe/MgO/Fe tunneling junctions by local tunneling

W. Wulfhekel[1], *M. Klaua*[1], *R. Urban*[2], *T. Monchesky*[2], *D. Ullmann*[1], *F. Zavaliche*[1], *J. Barthel*[1], *J.F. Cochran*[2], *B. Heinrich*[2], *and J. Kirschner*[1]

[1] *Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle*

[2] *Physics Department, Simon Fraser University, Burnaby BC, Canada V5A 1S5*

The performance of tunneling magnetoresistance junctions using amorphous barriers is governed by resonant tunneling through a large number of poorly understood defects in the barrier [1]. Tunneling proceeds by hopping, such that the intrinsic properties related to the band structure of the materials are washed away and the magnetoresistance is given by a momentum averaged spin-polarization of the electrons at the Fermi energy. In contrast to this, for perfect Fe/MgO/Fe junctions, a magnetoresistance of several hundred percents has been predicted due to band structure effects [2]. To study the intrinsic tunneling magnetoresistance, we have grown crystalline junctions by molecular beam epitaxy of MgO on single crystal Fe(100) substrates. Probing the oxide barrier by low energy electron diffraction, photoemission and scanning tunneling microscopy revealed high crystal perfection, a high tunneling barrier of 3.6eV and almost ideal layer-by-layer growth. Using scanning tunneling spectroscopy we find only a low density of localised defects in an otherwise homogeneous barrier. In a second step, crystalline Fe(100) top electrodes are deposited and spectroscopic mapping of structures is repeated revealing localised spots of higher conductance that we attribute to the defects in the buried MgO layers. Similar measurements have also been carried out using a conductive atomic force microscope in dynamic contact mode. We explain the ability to locally map defects in the buried oxide by a high fraction of ballistic electrons that transverse the Fe film and locally tunnel through the barrier. This is supported by an analysis of the shape of the I-V curves. Further, we present measurements on the magnetic properties of the tunneling structure.

[1] E.Y. Tsymbal and D.G. Petifor, Phys. Rev. B 58, 432 (1998)

[2] W. Butler, J. MacLaren, and X.G. Zhang, to be published

Theory of tunneling magnetoresistance of Fe/MgO/Fe and Co/Cu/vacuum/Co junctions

J. Mathon[1], *A. Umerski*[1], *and M. Villeret*[1]

[1] *Department of Mathematics, City University, London EC1V OHB, UK*

The tunneling magnetoresistance (TMR) of a junction with Fe(001) electrodes separated by an MgO epitaxial barrier is calculated from the real-space Kubo formula. The band structures of iron and MgO are described by tight-binding bands fitted to the *ab initio*

band structure of an iron overlayer on an MgO substrate. The dependence of the tunneling magnetoresistance ratio R_{TMR} on the thickness of the MgO barrier is determined. The polarization of electrons tunneling from iron to MgO is also calculated and discussed in terms of the band structures of the barrier and electrodes. The effect of a nonmagnetic metallic interlayer on the tunneling magnetoresistance will be also discussed. In particular, it will be demonstrated that the TMR due to tunneling between two Co electrodes separated by a vacuum gap remains nonzero when one of the electrodes is covered with a copper layer. This contradicts the classical theory of tunneling which predicts zero TMR. It will be shown that a nonzero TMR is due to spin-dependent quantum well states in the Cu layer which do not participate in transport. Finally the effect of interfacial roughness on TMR of a junction with a nonmagnetic metallic interlayer will be investigated using supercell simulation and CPA approximation for a single-band model of a tunneling junction.

Electronic Structure and Transport Properties of Tunnel Junctions

M. Freyss[1], *N. Papanikolaou*[1], *R. Zeller*[1], *and P.H. Dederichs*[1]
[1] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

We present ab-initio calculations for the electronic structure and transport properties of epitaxial Fe / I / Fe (001) tunnel junctions, where I is an insulating or a semiconducting barrier . The ground state properties are determined by the screened Korringa-Kohn-Rostoker Green's function method. This method scales linearly for layered systems, and allows for an exact treatment of the half-crystal geometry. For the transport properties we use a Green's function formulation of the Landauer formalism proposed by Baranger and Stone.

We focus on tunnel junctions with a ZnSe barrier. We show the ground state properties obtained for the two possible terminations of the interface, i.e with a Fe/Zn interface or a Fe/Se interface. We compare them to other barriers: Si, GaAs and MgO. In particular, we comment on the presence of Metal-Induced Gap States in the semiconductor, whose spin-polarization strongly depends on the nature of the barrier. We also present results for the magnetization profile, charge transfer and the $q_{||}$-resolved local density of states at E_F, emphasizing on the role of interface states. The spin-dependent transport properties are calculated for varying thicknesses of the barrier . We show that for large thicknesses the conduction through tunnel junctions can be understood in terms of the complex band structure of the bulk insulator. However, anomalies can occur due to surface states, in particular for symmetrical barriers and intermediate thicknesses, and then the conduction can be dominated by few resonant tunneling states.

Tunneling Magnetoresistance in Fe/MgO/Fe

P. Zahn[1] *and I. Mertig*[1]
[1] *Institut für Theoretische Physik, TU Dresden, Germany*

We use a Screened KKR method to calculate the electronic structure of a tunnel junction consisting of Fe electrodes separated by an insulating MgO barrier in a periodic superlattice structure selfconsistently. For the conductance the Landauer formula is evaluated in the ballistic limit as function of the magnetic configuration. Based on these conductances the TMR ratio is obtained.

We investigate the relation between TMR ratio and spin polarization of the electronic structure at the metal/insulator interface. To elucidate the microscopic origin of tunneling we introduce an effective tunneling density of states to illustrate localazation and angular momentum character of the tunneling states.

Ab initio calculations of tunneling through MgO barriers on Fe(001)

D. Wortmann[1], *S. Heinze*[1,2], *G. Bihlmayer*[1], *S. Blügel*[1]
[1]*Institut für Festkörperforschung des Forschungszentrums Jülich, 52425 Jülich*
[2]*Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg*

The tunnel-magneto resistance (TMR) effect has been extensively studied in the last couple of years. Due to the complicated interplay between electronic structure, atomic structure and the tunneling process through oxidised metal films there has been little theoretical work. The formation of the interface seems to be of great importance for the transport properties. Thus the spin-polarized STM, attracting much attention recently, might be an appropriate tool to study the correlation between oxide layers and the polarisation of the tunneling current.

In this poster we present our calculations of the electronic and magnetic structure of MgO/Fe(001) interfaces. We study two different systems: The Fe(001)/MgO/Fe(001) heterojunctions and the vacuum/MgO/Fe(001) arrangement. For the latter, the MgO/Fe(001) interface is studied in two different registries: Mg or O above the Fe atom. Different MgO thicknesses are taken into account. The current and its polarisation is related to the local density of states. We also analyze which states will contribute to the tunneling of heterojunctions.

Magneto-optical properties of multilayer- and surface layer systems

H. Ebert[1], *T. Huhne*[1]
[1] *Institut für Physik. Chemie, Universität München,*
Butenandtstr. 5-13, 81377 München, Germany

Magneto-optical spectra of magnetic solids in the visible regime provide a lot of information which enable one a deep insight into the electronic structure. While the corresponding experimental measurements are relatively easy to carry out, the interpretation of the spectra is quite complicated because of the interference of the effects of many electronic transitions involved. For this reason, the theoretical calculation of magneto-optical ef-

fects on the basis of ab-initio bandstructure calculations is an important means for the decoding of the experimental data.

Our method for the calculation of the frequency dependent, layer resolved optical conductivity for multilayer and surface layer systems, which has been presented earlier, allows to deduce all experimentally observable magneto-optical quantities. It is based on the self-consistent ab-initio Green's function method (KKR-GF).

The program has been extended for the use of the Tight-Binding KKR-method which enables us to treat more realistic, larger layer systems of up to 30 perturbed layers.

We present results for bulk Fe, Co, and Ni, as well as Au/Fe and Cu/Co surface layer systems which are, as far as possible, compared with the results of other authors and the experiment.

Transmission coefficients - a new formalism

I. Riedel[1], *P. Zahn*[1], *I. Mertig*[1]
[1] *Institut für Theoretische Physik, TU Dresden, Germany*

A new formalism to calculate the transmission coefficients of electrons from a material A through an arbitrary metallic, semiconducting or insulating barrier B is presented. The transmission coefficients are derived from the electronic structure of a periodic A/B superlattice. The electronic structure of such a multilayer is calculated selfconsistently within a Screened Korringa-Kohn-Rostoker method.

The new formalism can be understood as an extended Kronig-Penney model: Starting from an arbitrary anisotropic electronic structure of the periodic multilayer A/B, the transmission coefficients through a single barrier B can be derived for all states of material A. First applications to the calculation of the transmission coefficients of Cu electrons through ferromagnetic Fe and Co barriers are presented.

Spin injection

G. Schmidt

Spin accumulation and Andreev reflection in ferromagnetic wires

W. Belzig[1], *A. Brataas*[1], *Yu. V. Nazarov*[1], *and G.E.W. Bauer*[1]
[1] *Delft University of Technology, The Netherlands*

Mesoscopic heterostructures of ferromagnets (F) and superconductors (S) currently attract a lot of interest. Transport in these system faces the problem of conversion of a spin polarized current in F into a spinless supercurrent. Many important phenomena, such as spin relaxation or spin dependent interface scattering, can therefore be investigated. We have formulated kinetic equations based on a Green's function approach to study transport in FS-heterostructures and applied it to an F-wire connected to an S-lead.

The interplay between Andreev reflection and spin-accumulation crucially determines the resistance of the system. For example the resistance change due to S is positive at bad interfaces, but at moderately clean interfaces can be decreased by an amount larger that in the unpolarized case. Recent experimental results are shown to coincide with our theory.

Giant Magnetoresistance in hybrid superconductor/ferromagnetic sandwich heterostructures

A. Vedyayev[1], *N. Ryzhanova*[1], *B. Dieny*[2], *C. Lacroix*[3], *N.Strelkov*[1], *and D.Bagrets*[2]

[1] *Moscow Lomonosov State University, Moscow, 119899, Russia*

[2] *CEA/Grenoble, DRFMC, SP2M/NM, 38054 Grenoble, France*

[3] *Laboratorie de Magnétisme Louis Néel, CNRS, BP166, 38042 Grenoble France*

The electron transport through the one and two-domain ferromagnetic metal (F) in contact with superconductor (S) is investigated theoretically. The conductance is calculated in Kubo formalism with Green functions found as the solutions of the Gorkov equations. It is shown that Giant magnetoresistance (GMR) defined as a relative difference of the conductivities for one and two domain samples behaves differently in the ballistic and diffuse regimes. For the first one, the value of GMR is sufficiently high and for the latter one in the limit of the strong electron scattering GMR almost vanishes. The interpretation of this behaviour is given comparing the contributions to the total resistance of the system from Andreev reflection on F/S and usual quantum reflection on F/F interfaces.

A study of conductance oscillations in mesoscopic Andreev interferometers in the presence of spin orbit coupling

C. Newman[1] *and C.J. Lambert*[1]

[1] *Department of Physics, Lancaster University, Lancaster LA1 4YB, U.K.*

We present an investigation into conductance oscillations in mesoscopic Andreev interferometers in the presence of spin orbit coupling. It is known that when two superconducting islands are embedded in a diffusive metal the 2-probe conductance exhibits oscillations as a function of the phase difference $\Delta\phi$ in the order parameters of the two superconductors provided that the relevant length scale exceeds the spacing between the two superconductors [1]. If one includes spin orbit coupling then those oscillations are expected to persist but with a reduced amplitude.

To confirm this prediction we solve the generalized Bogoluibov – de Gennes equation in the presence of spin-orbit coupling using a recursive Green's function technique, and compute the conductance within a multiple-scattering approach. Results are presented for the conductance of a ballistic metal with three different magnetic configurations, namely: a normal non-magnetic strip, a ferromagnetic strip and an antiferromagnetic strip, all containing two superconducting islands and a potential barrier.

[1] N.K. Allsopp et al., J.phys.: Condens. Matter 8, L377 (1996).

Correlation effects on spin-polarization in transition metals

A. Lichtenstein

Ab-initio electronic structure study of materials used in the TMR

Arthur Ernst[1]

[1] *Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle*

Ab-initio studies of electronic structure of materials, which are used in the Tunnel Magnetoresistance (metallic electrodes, semiconducting or insulating barriers), entail great difficulties involved by treatment of excitation energies and many-body effects. The most successful first principles method, the density functional theory (DFT) within the local density approximation (LDA), is designed for ground state properties and can not provide proper description of band structure of semiconductors and insulators. It is possible to calculate accurately from first principles the quasiparticle energies and band gaps by solving the Hedin's set of equations for the full Green's function in the random-phase approximation (GW approximation). Here we present preliminary calculations of some semiconductors with a realization of the GWA based on the Korringa-Kohn-Rostoker (KKR) method.

Quasiparticle calculations for CaB_6

P.J. Kelly[1], *E.J. Tromp*[1], *P. van Gelderen*[1,2], *G. Brocks*[1], *and P.A. Bobbert*[3]

[1] *University of Twente, The Netherlands*

[2] *Catholic University of Nijmegen, The Netherlands*

[3] *Eindhoven University of Technology, The Netherlands*

Current proposals to explain the recently observed high temperature magnetism of La-doped CaB_6 depend on peculiarities of the electronic structure as they are known from local-density-approximation (LDA) calculations. We present the results of parameter-free quasiparticle calculations of the single-particle excitation spectrum for stoichiometric CaB_6. We discuss how the improved treatment modifies the LDA electronic structure, the consequences for understanding the basic properties of the recently discovered ferromagnetic phase of $La_xCa_{1-x}B_6$, and the implications for applications.

A review of theoretical approaches to CMR in Manganites

J. van den Brink[1]

[1] *University of Twente, The Netherlands*

We give a short review of the current theoretical approaches to explain the collosal magnetoresistance in doped manganites and discuss lattice, spin and orbital degrees of freedom, which all play an important role in the physics of manganese oxides. Special attention is

paid to the recent proposal that in the metallic systems an ordering of cubic, complex, orbitals may take place [1].

[1] Jeroen van den Brink and Daniel Khomskii "Novel type of orbital ordering: Complex orbitals in doped Mott insulating manganites" Submitted to Phys. Rev. Letters.

Experimental results on spin polarized tunneling

A. Fert[1]

[1] *Unit Mixte de Physique CNRS-Thomson and Universit Paris-Sud, 91404 Orsay (France)*

The first part of the talk will be devoted to experiments aimed at clearing up the physical mechanism governing the spin polarization of tunneling electrons in magnetic tunnel junction. Most of our experiments have been performed on junctions in which a half-metallic electrode ($La_{0.7}Sr_{0.3}MnO_3$ = LSMO) is used to analyse the tunneling probability spin polarization of the electrons tunneling from or into the ferromagnetic transition metal (Co, Fe or NiFe) of the counter-electrode. We find that the amplitude and sign of the spin polarization of a given ferromagnetic metal depend on the choice of the insulating material of the barrier. For example, the spin polarization of Co is **positive** (that is tunneling probability higher for majority spin electrons) when the barrier is $\mathbf{Al_2O_3}$ **(ALO)** and **negative** when it is $\mathbf{SrTiO_3}$**(STO)** or $\mathbf{CeLaO_x}$**(CLO)**[1, 2]. This is consistent with recent calculations which emphasize the important role of the bonding mechanism at the metal/oxide interface in determining the spin polarization[3, 4]. The importance of the interface effects is confirmed by experiments which show that the polarization of Co in Co/STO/LSMO junctions becomes positive when an ultra-thin ALO layer is intercalated between Co and STO. Calculations for various types of metal/oxide interface would be of great interest.

In the second part of the talk I will discuss the issue of the temperature dependence of the tunnel magnetoresistance (TMR) in junctions with electrodes of half-metallic oxide. The TMR of LSMO/STO/LSMO junctions is very high at low temperature (450%) but vanishes at about 200K, well below the Curie temperature of LSMO ($T_c \approx 350$K). It has been argued that this could be due to the intrinsic temperature dependence of the spin polarization at the interfaces of a double-exchange oxide. However the TMR of our Co/STO/LSMO junctions vanishes only at about T_c, which suggests that the temperature dependence of the TMR should be rather related to extrinsic roughness effects. This would be a good news for the prospect of high TMR at room temperature with half-metallic oxides having a relatively high T_c. I will discuss some experimental results obtained with $Fe_3O_4$and double perovskites like Sr_2FeMoO_6.

1. J.M.De Teresa, A.Barthlmy, A.Fert, J.P.Contour, R.Lyonnet, F.Montaigne, P.Seneor, A.Vaurs; Phys. Rev. Lett. 82, 4288 (1999)

- J. M. De Teresa, A. Barthlmy, A. Fert, J-P. Contour, F. Montaigne, P. Seneor, Science 286, 507 (1999).
- I.I. Oleinik, E. Y. Tsymbal, D. G. Pettifor, Phys. Rev. B62, 3952 (2000).
- E. Y. Tsymbal, I.I. Oleinik, D. G. Pettifor, J. Appl. Phys. 87, 5230 (2000).

Charge and spin degrees of freedom in ferromagnetic single-electron transistors

J. Barnaś[1], *J. Martinek*[2], *G. Michałek*[2], *and B.R. Bułka*[2]

[1] *Department of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland*

[2] *Institute of Molecular Physics, Polish Academy of Sciences, ul. Smoluchowskiego 17, 60-179 Poznań, Poland*

Interplay of charge and spin degrees of freedom in ferromagnetic single electron transistors (FM SET's) has been studied theoretically in the limit of incoherent sequential tunnelling. The device consists of a small central electrode (metallic grain, quantum dot, or an atom), which is coupled to two ferromagnetic metallic leads. The discrete energy spectrum of the central electrode plays a significant role When the intrinsic spin relaxation time is sufficiently long, the spin asymmetry in tunnelling rates for the electrons with opposite spin orientation can lead to spin accumulation. The formalism developed allows to calculate electric current, spin and charge accumulation, spin and charge fluctuations, and the tunnel magnetoresistance (TMR).

There are two different scales in all characteristics of the junction. When the charging energy E_c is significantly larger than the interlevel spacing ΔE, the shorter scale is related to the discreteness of energy spectrum and the longer one to the discrete charging of the grain (dot) with single electrons. The features due to discrete energy levels can be seen then at low temperatures and disappear relatively quickly with increasing temperature; much faster than the features due to discrete charging. It is shown that spin accumulation gives rise to TMR and discrete charging leads to oscillations in TMR.

The junction characteristics are periodic functions of the gate voltage. At low temperatures the periods are twice as long as the corresponding ones at high temperature. This is because at low temperatures the situations with even and odd numbers of electrons on the island can be distinguished, while at high temperatures this difference disappears.

Giant Asymmetry of Current And of Tunnel Magnetoresistance in Double Barrier Junctions

M. Chshiev[1], *D. Stoeffler*[1], *A. Vedyayev* [1,2], *and K. Ounadjela*[1]

[1] *IPCMS (UMR 7504 CNRS-ULP) - 23 rue de Loess,F-67037 Strasbourg cedex, France*

[2] *Moscow Lomonosov State University, Moscow, 119899, Russia*

A quantum theory of the tunnel magnetoresistance (TMR) in the asymmetric magnetic double barrier structures of the form $M/O_1/M/O_2/M$ is presented (M and O are the magnetic metal and oxide layer respectively). The thicknesses or heights of O_1 and O_2 barriers are different. Formation of quantum well states in the middle metallic layer gives rise to resonances in currents and TMR. Under applied voltage the positions of the resonant levels are shifted and for considered asymmetric structure this shift is different for the direct and inverse bias voltage. As a result I-V curve of the structure is highly asymmetric, demonstrating the diode behaviour. The characteristics of these "diode" is sensitive to the applied magnetic field.

Parameter-free calculations of spin dependent transport

K. Xia[1], *M. Zwierzycki*[1,2], *P.J. Kelly*[1], *G.E.W. Bauer*[2],
I. Turek[3], *J. Kudrnovský*[4], *and V. Drchal*[4]
[1] *University of Twente, The Netherlands*
[2] *Delft University of Technology, The Netherlands*
[3] *Academy of Sciences of the Czech Republic, Brno*
[4] *Academy of Sciences of the Czech Republic, Prague*

Electronic transport through layered structures can best be formulated in terms of scattering theory in which the scattering matrix plays a key role. We calculate from first-principles the spin-dependent scattering matrix for hybrid structures comprising ferromagnetic and non-magnetic materials using the very efficient TB-LMTO method. The method is applied to GMR and JMR. For non-collinear magnetic configurations, the spin-mixing conductance can be much larger than the normal conductance when the contact resistance is very high. The effect of disorder is discussed.

Ab initio calculations of tunneling magnetoresistance

M. Zwierzycki[1,2], *K. Xia*[2], *P.J. Kelly*[2], *G.E.W. Bauer*[1],
I. Turek[3], *J. Kudrnovský*[4], *and V. Drchal*[4]
[1] *Delft University of Technology, The Netherlands*
[2] *University of Twente, The Netherlands*
[3] *Academy of Sciences of the Czech Republic, Brno*
[4] *Academy of Sciences of the Czech Republic, Prague*

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 we can treat both specular and diffuse scattering on an equal footing.

Spin-dependent electron tunneling through planar junctions revisited

J. Henk

Hot spots in tunneling magnetoresistance

V. Drchal[1]
[1] *Institute of Physics, AS CR, Praha, Czech Republic*

The calculations of tunneling across the magnetic multilayers with an insulating spacer revealed small regions in the surface Brillouin zone with high transmittance, the so-called hot spots, that give important contribution to conductance and which lead to considerable numerical difficulties. The results of a closer analysis based on the transfer matrix method will be discussed with the aim to explain their origin.

Effects of Interface States on Tunneling: A Simple Model

O. Wunnicke[1], *N. Papanikolaou*[1], *and P.H. Dederichs*[1]
[1] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

We present a simple model to discuss the effects of interface states on the tunneling conductance. The model consists of two semiinfinite crystals seperated by a constant potential barrier. The Bloch states in the crystals are described in the nearly-free-electron model by including the Fourier coefficients of the bulk potentials. The wavefunctions in the crystal and in the vacuum are matched at the interface plane. Surface states are introduced by a negative δ-potential at the interfaces. The model has the advantage that the reflection and transmission coefficients can be calculated analytically, although in practice the linear equations resulting from the matching condition are solved numerically.

While in the one-band model the surface states are localized and do not contribute to the conduction, in the multi-band case these states become resonant and lead to sharp peaks in the conductance, which in a $\vec{q}_{\|}$-resolved conductance-plot are localized on lines close to the edges of the 'new' bands.

For a symmetrical barrier the resonances on both sides of the barrier split into bonding and antibonding peaks due to the overlap of the localized wave functions. Then at the resonance condition full transmission is observed, so that the incoming wave is not attenuated. If the natural halfwidth of the single resonance is larger than the splitting, this resonant tunneling effect becomes less effective and attenuation sets in. The model calculation explains, why for intermediate barrier thicknesses the surface resonances can dominate the conductance and the normal exponential decay is only observed for larger thicknesses. We discuss the importance of this effect in tunneling junctions.

Topics in the CPP transport in multilayers

J. Kudrnovský[1,3,4], *V. Drchal*[1,4], *I. Turek*[2,4], *P. Bruno*[3], *and P. Weinberger*[4]
[1] *Institute of Physics AS CR, Praha, Czech Republic*
[2] *Institute of Physics of Materials AS CR, Brno, Czech Republic*
[3] *Max-Planck Institut für Mikrostrukturphysik, Halle, Germany*
[4] *CMS, University of Technology, Vienna, Austria*

We will discuss three different problems related to the perpendicular transport in metallic magnetic multilayers, namely:

(a) Justification of the interatomic view of the *ab inito* transport in metallic alloys and multilayers by evaluating the resistivity of bulk fcc-AgPd alloy and its comparison with both experiment and KKR-CPA calculations;

(b) Study of the combined effect of two types of disorder, namely the substitutional disorder (interdiffusion at interfaces) and of the 'structural' disorder (thickness fluctuations of magnetic and/or spacer layers in the magnetic multilayer); and

(c) Tunneling magnetoresistance across the vacuum barrier, in particular some practical attempts how to overcome the problem of the so-called hot-spots on a computational level.

GMR in Co/Cu and Fe/Cr multilayers – a comparison

J. Binder[1], *P. Zahn*[1], *and I. Mertig*[1]
[1] *Institut für Theoretische Physik, TU Dresden, Germany*

Full ab initio calculations for the giant magnetoresistance (GMR) in Co/Cu and Fe/Cr multilayers are presented. The electronic structure of the multilayers is calculated by spin density functional theory using a Screened Korringa-Kohn-Rostoker method. Scattering of impurity atoms in the multilayers is described by means of a Green's-function method. The scattering potentials are calculated self-consistently. The transport properties are treated quasi-classically solving the Boltzmann equation including the electronic structure of the layered system and the anisotropic scattering. The solution of the Boltzmann equation is performed iteratively taking into account both scattering out and scattering in terms (vertex corrections). Furthermore the influence of interface scattering is incorporated by averaging the scattering cross sections of different impurities at various sites in the supercell.

It will be shown that there is an excellent agreement of experimental and numerical results concerning the general trend of GMR in Co/Cu systems depending on the type and the

position of impurities. The increase of GMR when impurities are placed within the Co layer and not at interface is directly connected to the quantum confinement in magnetic multilayers. In contrast, the GMR in Fe/Cr multilayers is attributed to spin-dependent interface scattering, especially to the strong spin dependence of electron scattering at chromium impurities in the Fe interface layer. The spin asymmetry of the Fe/Cr interface is crucial and determines the magnitude of GMR.

Enhancement of GMR due to spin mixing in magnetic multilayers with superconducting contacts

C.J. Lambert[1], *and F. Taddei*[1]
[1] *Department of Physics, Lancaster University, Lancaster LA1 4YB, U.K.*

We study giant magnetoresistance (GMR) in magnetic multilayers with a single superconducting contact in the presence of spin mixing processes. It has recently been shown[1] that when spin-flip processes are absent, the GMR ratio of magnetic multilayers is strongly suppressed by the presence of a superconducting contact. Here we demonstrate that GMR can be dramatically enhanced by spin-orbit scattering and/or non-collinear magnetic moments. The system is described using a tight binding model with either s-p-d or s-d atomic orbitals on each site. In contrast with the magnetoresistance in the presence of normal contacts, where the resistance varies monotonically as the angle between the magnetic moments of successive layers varies from zero to pi, we find that the resistance in the presence of a superconducting possesses an extremum at intermediate angles.

[1] F. Taddei, S. Sanvito, J.H. Jefferson and C.J. Lambert, Phys. Rev. Lett., **82** 4938 (1999)

Electrical transport properties of bulk Ni_cFe_{1-c} alloys and related spin-valve systems

C. Blaas[1], *L. Szunyogh*[2], *P. Weinberger*[1], *C. Sommers*[3], *P. M. Levy*[4]
[1] *Center for Computational Materials Science, Technische Universität Wien, Austria*
[2] *Department of Theoretical Physics, Technical University Budapest, Hungary*
[3] *Laboratoire de Physique des Solides, Université de Paris-Sud, Orsay, France*
[4] *Department of Physics, New York University, New York, USA*

Within the Kubo-Greenwood formalism we use the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method together with the coherent-potential approximation for layered systems to calculate the resistivity for the permalloy series Ni_cFe_{1-c}. We are able to reproduce the variation of the resistivity across the entire series; notably the discontinuous behavior in the vicinity of the structural phase transition from bcc to fcc. The absolute values for the resistivity are within a factor of two of the experimental data. Also the giant magnetoresistance of a series of permalloy-based spin-valve structures is estimated; we are able to reproduce the trends and values observed on prototypical spin-valve

structures.

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

B.Yu. Yavorsky[1] *and I. Mertig*[1]
[1] *Institut für Theoretische Physik, TU Dresden, Germany*

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.

Current Induced Interlayer Coupling

P.M. Levy[1], *C. Heide*[1], *S. Zhang*[2], *A. Fert*[3]
[1] *Department of Physics, New York University, Washington Place, New York, NY 10003*
[2] *Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211*
[3] *Unite Mixte de Physique, LCR-Thomson, 91404 Orsay, France*

It has recently been shown that a perpendicular current in a magnetically multilayered structures induces an unusual bilinear coupling between the magnetizations of the layers. While this was demonstrated in the ballistic regime, transport is likely to be diffusive in the structures where this may be relevant to the role of currents in switching the magnetization of the layers. We have derived the current induced coupling by using the Boltzmann equation in terms of the parameters used to describe the giant magnetoresistance of magnetically layered structures, and thereby estimate the strength of this coupling.

Current-induced switching

C. Heide[1] *and P.M. Levy*[1]
[1] *Department of Physics, New York University, 4 Washington Place,New York, NY 10003*

The switching of magnetic layers is studied under the action of a spin current in a ferromagnetic metal/non-magnetic metal/ferromagnetic metal spin valve. We find that a

large contribution to the switching comes from the non-equilibrium exchange interaction between the ferromagnetic layers. This interaction defines the magnetic configuration of the layers with minimum energy and establishes the threshold for a critical switching current. Depending on the direction of the critical current, the interaction changes sign and a given magnetic configuration becomes unstable. To model the time dependence of the switching process, a set of coupled Landau-Lifshitz equations is derived for the ferromagnetic layers. Higher order terms in the non-equilibrium exchange coupling allow the system to evolve to its steady-state configuration. In addition, spin-flip processes can excite oscillations in the magnetization as the spin-current relaxes and transfers angular momentum to the local moments via electron-magnon scattering processes. These oscillations effectively reduce the coercivity of the layer, however, cannot in general lead to switching by themselves.

Experiments of magnetization reversal by spin injection

A. Fert[1]

[1] *Collaboration between Unite Mixte de Physique at Orsay, L2M-CNRS Lab at Bagneux and Universite de Brest*

Our experiments are performed on Co/Cu/Co trilayered pillars of submicronic size fabricated by e-beam lithography. The magnetic configuration can be switched from parallel (P) to antiparallel (AP) by injecting electrons from the thin Co layer to the thick one, and from AP to P by a current in the opposite direction. The switching is detected by GMR and we have studied the dependence of the switching currents as a function of the applied field. I willl present a numerical fit of our results with Slonczewski's model and with another type of model based on spin acumulation effects.

Current-Induced Torques in Ferromagnetic Nanostructures

N. Pattinson[1] *and C.J. Lambert*[1]

[1] *Department of Physics, Lancaster University, Lancaster LA1 4YB, U.K.*

Recent experimental work on Co/Cu/Co structures [1] has shown that a spin-polarized current can flip the magnetic moment in a ferromagnetic metal. This observation agrees with earlier theoretical predictions [2] that a spin-polarized current exerts a torque at the interface between a magnetic and non-magnetic material. Using a simple s-band tight-binding Hamiltonian, we examine the torque, due to an incoming spin-polarized current, by rotating the magnetic moment of the ferromagnetic island. Using numerical scattering methods, the torque is calculated from the incoming and outgoing fluxes of spin angular momentum. Results are obtained for a clean normal-ferromagnetic-normal system and for a normal-ferromagnetic-superconductor system. It is found that switching on superconductivity in one of the leads can either increase or decrease the torque. This leads us to conclude that turning on superconductivity can flip the magnetic moment of the island.

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

[2] J.C. Slonczewski, J.Magn.Magn.Mater, 159 L1(1996)

Electronic structure of Co-Alumina tunnel junctions

E. Tsymbal

Perpendicular transport in Fe/Ge heterostructures

P. Weinberger[1], *L. Szunyogh*[2], *C. Blaas*[1], *C. Sommers*[3], *and P.M. Levy*[4]

[1] *Center for Computational Materials Science, Technische Universität Wien, Austria*

[2] *Department of Theoretical Physics, Technical University Budapest, Hungary*

[3] *Laboratoire de Physique des Solides, Université de Paris-Sud, Orsay, France*

[4] *Department of Physics, New York University, New York, USA*

Based on the Kubo-Greenwood formalism as adapted to layered systems an approach is discussed that allows us to separate the resistance of the current leads from that of the region whose resistance we wish to calculate for current perpendicular to the plane of the layers. By applying this approach to Fe/Ge/Fe structures we find that at least 9 layers of the magnetic electrodes should be included in the calculation in order to perform such a separation. With different structures in the Ge-spacer part, we find that the concentration of vacancies plays a crucial role for the existence of a sizeable magnetoresistance (MR), while the actual structure in the spacer seems to be of less importance. Depending on the type of structure and the number of spacer layers (in a typical regime of 6–21 layers) the MR for ordered structures varies between 35% and 45%. Vacancy concentrations of more than 10%, however, wipe out the MR completely. Interdiffusion at the Fe/Ge interfaces produces very similar effects.

Resolving Complex Atomic-Scale Spin-Structures by SP-STM

D. Wortmann[1], *S. Heinze*[1,2], *Ph. Kurz*[1], *G. Bihlmayer*[1], *and S. Blügel*[1]

[1] *Institut für Festkörperforschung, Forschungszentrum Jülich, D–52425 Jülich*

[2] *Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg*

We propose the application of the topography mode of a spinpolarized scanning tunneling microscope (SP-STM) to investigate the complex atomic-scale magnetic structure of otherwise chemically equivalent atoms. We extend the model of Tersoff and Hamann to the case of a spinpolarized tip with an arbitrary magnetization direction and a sample with an arbitrary magnetic structure. We demonstrate the potential of this approach by applying it to resolve complex collinear and non-collinear magnetic surface structures. Several examples will be presented: Among them are a monolayer Cr on a Ag(111)-substrate, which exhibits a coplanar non-collinear periodic Néel state, and a three dimensional non-collinear magnetic structure of a Mn-monolayer on a Cu(111)-substrate. The magnetic

ground-states of Cr/Ag(111) and Mn/Cu(111) have been found on the basis of *ab initio* vector spin-density total-energy calculations. A further example of the successful application of the SP-STM is the mapping of the antiferromagnetic ordering of a monolayer of Mn on a W(110)-substrate as reported recently in Science (**288**,1805(2000)).

Magnetic properties of Co/Cu/Ni trilayer on the Cu(100) surface

I.A. Abrikosov[1], *E.I. Isaev*[2], *L.V. Pourovskii*[1,2],
A.M.N. Niklasson[3], *Yu.Kh. Vekilov*[2], *and B. Johansson*[1]
[1] *Condensed Matter Theory Group, Physics Department,*
Uppsala University, S-75121 Uppsala, Sweden
[2] *Theoretical Physics Department, Moscow State Institute of Steel and Alloys,*
Leninskii pr., 4, 117936 Moscow, Russia
[3] *Theoretical Division and Center for Materials Science,*
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Magnetic moments and total energies have been calculated for $Co_3/Cu_N/Ni_5$ trilayers and Cu_N/Ni_5 bilayers on the Cu(100) surface by means of the interface Green's function technique within the basis set of linear muffin-tin orbitals. We observe that there are two distinct energy scales in this system, the energy difference between the ferromagnetic and the paramagnetic samples, and the substantially smaller energy difference between the ferromagnetic sample and the sample there only Ni layers are paramagnetic, while Co layers have nonvanishing magnetic moments. This observation is in agreement with recent experiment by Ney *et al.* (Phys. Rev. **B 59** 3938 (1999)) where there was observed that the magnetization of Co and Ni layers vanishes at different temperatures. We find that Co and Ni layers in the trilayer are exchange coupled. The coupling is oscillatory and decreases with increasing number N of the spacer Cu layers. Magnetic moment profiles were calculated and discussed. We find very good agreement between the theory and the experiment for the trilayers, but large deviations are found for the bilayers. This we explain by a possibility of a formation of complicated magnetic structures within the Ni films in the absence of Co layers.

Electronic and magnetic properties of ferromagnet-semiconductor heterostructure systems

A.Ya. Perlov[1], *H. Ebert*[2], *I. Cabria*[2], *M. Košuth*[2], *and V. Crisan*[2]
[1] *Max-Planck Research Group, 'Theory of Complex and Correlated Electron Systems',*
D-01062 Dresden, Germany
[2] *Institut für Physikalische Chemie, Universität München,*
Butenandtstr. 5-13, D-81377 München, Germany

The electronic and magnetic properties of ferromagnet-semiconductor (FM/SC) heterostructure systems have been studied by means of fully relativistic LMTO as well as scalar-relativistic KKR-CPA band structure calculations. The structural model used for our

calculations was proposed by McLaren and coworkers. In contrast to the work of these authors periodic multi-layer systems have been studied, taking for the ferromagnet Fe and for the semiconductor Ge and GaAs, respectively. In addition the influence of impurities in the ferromagnetic subsystem and the effect of interdiffusion at the interface was investigated. Concerning the resulting magnetisation profiles the most important features are that no magnetically dead layers occurred and an appreciable induced magnetisation was found in the semiconductor subsystem.

To initiate corresponding experimental work the magnetic circular dichroism has been investigated for the $L_{2,3}$-absorption spectra of Ga as well as As. In all cases the circular dichroism was found to be pronounced enough to be detectable.

Investigations on the magneto-crystalline anisotropy energy revealed that all of the studied systems should show a perpendicular anisotropy. Calculations of the spin-orbit induced orbital magnetic moment in a spin-resolved way allowed to check the correlation of this quantity with the magneto-crystalline anisotropy energy. It was found that the relationship suggested recently by van der Laan is quite well fulfilled.

The theory of GMR and TMR in segmented magnetic nanowires with surface roughness

M. Ye. Zhuravlev[1,2], *H.O. Lutz*[1], *A.V. Vedyayev*[3]

[1] *Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld 1, Germany*

[2] *on leave from N. S. Kurnakov Institute of General and Inorganic Chemistry of the RAS, 117907 Moscow, Leninskii prosp., 31, Russia*

[3] *Department of Physics, Moscow State University, Moscow, 119899, Russia*

We have developed a Green function-based quantum statistical approach to the GMR in layered nanowire, including spin-dependent diffusive surface scattering. We have constructed the Green-function and calculated the resistivity and the GMR of the nanowire. The interplay between the spin-dependent electron scattering in the bulk and the surface leads to a complex behaviour of the GMR as a function of nanowire radius and surface potential strength. Our approach reproduces the size effect obtained in the quasiclassical theories. Resistivity and GMR have been found to oscillate due to the quantization of the electron motion in the direction perpendicular to the wire axis. The developed theory of GMR in segmented nanowire explains the experimentally observed changes in GMR in the nanowires comparing with laterally infinite multylayers.

Fermi surface flattening effects on magnetic interlayer coupling

E. Holstrom

5 News from the TMR2 Network

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

5.1 Workshop/Conference Announcements

5.1.1 Workshop on Physics of f-Electron Systems

Daresbury (UK) 6-8 April 2001
Sponsored by ESF & TMR2

Motivation

The workshop will focus on f-electron systems, and will aim at creating a forum for discussions between experimentalists and theoreticians, and among theoreticians between ab-initio band structure practisioners and many body theoreticians.

Scientific content

The Workshop will concentrate on three main themes:

A) The strengths and limitations of DFT based total energy schemes, including self-interaction corrections, orbital polarization and LDA+U.

B) Many-body treatment of f-electrons, including the implementation of Dynamical Mean Field Theory in 'ab-initio' schemes.

C) New experimental developments for rare earth and actinide systems.

Invited Speakers

The preliminary list of speakers is as follows ($\star$ confirmed; $\circ$ contacted, $-$ to be contacted)

∘A. Georges, France,
⋆J. Lægsgaard, Denmark,
⋆G. Lander, Germany,
⋆P. Wachter, Switzerland,
⋆Z. Henkie, Poland,
⋆P. Oppeneer, Germany,
⋆L. Petit, Denmark,
⋆M. Brooks, Germany,
⋆P. Söderlind, USA,
∘S.Y Savrasov or G. Kotliar, USA,
⋆V. Antonov, Ukraine,
⋆T. Gouder, Germany,
∘B. Johansson, Sweden,
∘U. Lundin, Sweden.

Participation

If you are interested to participate and contribute a paper please contact Damian Jones (d.r.jones@dl.ac.uk). A registration fee of £50 is requested. Limited financial support could be available.

Organisers:

- Olle Eriksson
  Department of Physics, Uppsala University, Sweden
  Phone: +46 (0)18-4713625, Fax: +46 (0)18-4713524,
  `olle.eriksson@fysik.uu.se`
- Axel Svane
  Institute of Physics and Astronomy, University of Århus, Denmark
  Phone: +45-8942-3678, Fax: +45-8612-0740,
  `svane@ifa.au.dk`
- Walter Temmerman
  Daresbury Laboratory, UK
  Phone: +44-1925-603227, Fax: +44-1925-603634,
  `W.M.Temmerman@dl.ac.uk`

6 News from the ESF Programme

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

6.1 Reports on Workshops/Conferences

6.1.1 Report on CMS2000

10th Computational Materials Science Workshop Villasimius, Sardinia, Italy, 7-12 September 2000

The tenth edition of the Computational Materials Science Workshop (CMS2000) has been held successfully in Villasimius, Sardinia, Italy on 7 to 12 September 2000. The workshop has been funded by the European Union under the *High-Level Scientific Conferences* programme, by the European Science Foundation under the program *Electronic structure calculations for elucidating the complex atomistic behaviour of solids and surfaces*, by the University of Cagliari, and the National Institute for the Physics of Matter.

A total of 89 participants took part in the event. Almost all of them (96%) were scientists active in EU countries or associated states. The number of participants (of any nationality) active in the various represented countries was as follows: Italy 31; Germany 17; U.K. 7; France 7; Sweden 5; Switzerland 4; Brasil 4; Finland 3; Belgium 3; Spain 3; Netherlands 2; Austria 1; Czech Republic 1; Ukraine 1, USA 1. The pleasant environment and reasonably good weather helped the integration among participants.

The scientific activities consisted of 8 oral sessions comprising 20 invited lectures (1 hours each), and of two distinct poster sessions, comprising 30 posters each. The (one-hour or three-hour) invited lectures were centered on both basic issues and applications of ab initio methods, prevailingly density-functional based. *A. Baldereschi* (EPF Lausanne, Switzerland) discussed recend advances in the understanding of electronic structure of adsorbates on metals. *S. Baroni*, (SISSA Trieste, Italy) reviewed the very successful linear response theory of dielectric and dynamical properties of solids, and a novel ab initio theory of magnons. *S. Fahy* (Cork University, Ireland) gave a compelling review of the present state of the art in Quantum Montecarlo. *R. O. Jones* (KFK Jülich, Germany)

addressed in detail the limits of different DFT exchange-correlation functionals in his talks on clusters, polymers and anomalous-thermal-expansion materials. *M. Parrinello* (MPI-FF Stuttgart, Germany) covered the recent work of his group on Ziegler-Natta catalysis and NMR shifts in organics *R. Resta* (Università di Trieste, Italy) reinterpreted his own seminal work on dielectric polarization in the light of the generalized position operator, and presented applications to electronic localization in dielectrics. *M. Scheffler* (Fritz-Haber-Institut Berlin, Germany) covered several topics relevant to the growth of semiconductor nanostructures and catalytic activity on metal surfaces. Finally, two experimental talks completed the picture: *O. Ambacher* (WSI-TU Munich, Germany) reviewed very recent experimental evidences and effects of macroscopic polarization effects in nitride nanostructures, and *J. Frenken* (Leiden University, The Netherlands) discussed an intriguing case of in-surface diffusion mediated by vacancies, and the exciting prospects of nanotribology with the STM.

Last-minute changes to the oral invited program were fairly substantial. Quite unfortunately, A. Zunger (NREL) had to cancel his participation a week before the event. Even more regrettably, U. Landman (Georgia Tech) simply did not show up at the conference. M. Parrinello kindly agreed to cover part of the time thus freed up.

The poster sessions collected about 60 distinct original contributions from participants. The titles of the contributions are collected on the web site of the conference, `http://www.dsf.unica.it/CMS2000`. Papers related to both contributed and invited talks will be published in a special issue of Computational Materials Science in 2001.

6.2 Reports on Collaborative Visits

Report on a Collaborative Visit of Adam Kiejna (Uniwersity of Wrocław) to Prof. Matthias Scheffler (Fritz-Haber-Institut MPG, Berlin)

4 – 6 December, 2000

I visited Professor Matthias Scheffler and his group at the Fritz-Haber-Institut der MPG in Berlin from 4 to 6 December, 2000.
The aim of my visit was to discuss with M. Scheffler, K. Reuter and V. Ganduglia-Pirovano the first principles calculations of oxygen adsorption on different metal surfaces. In particular, we have discussed similarities and differences between subsurface adsorption of oxygen at Al(111), done recently by myself with the pseudopotential plane-wave code, and the LAPW calculations for the O/Ru(0001) and O/Rh(111) systems performed at the FHI by K. Reuter and V. Ganduglia-Pirovano. This includes the character of bonding, destabilization of the surface due to subsurface oxygen, the relevance of different tests, and the possibilities for the metal-oxide formation.
We discussed with Matthias and the other members of his group some technical details of the fhi98md code and the progress in a collaborative project we are carrying out together on the alkali metal adsorption on Al surface.
I also had the opportunity to discuss oxygen adsorption on silver and other projects carried out in M. Scheffler's group.
Finally, I discussed the possibility of verification of some of my results for O/Al(111) and O/Mg(0001) systems with experimentalists from FHI.

Adam Kiejna

Report on collaborative visit of Magali Benoit (Laboratoire des Verres, University of Montpellier) to the University of Cambridge

September 25 - September 29, 2000

The purpose of my visit to Cambridge was to discuss about the general problems encountered in glasses and particularly in the silicate ones. I am currently starting an *ab initio* molecular-dynamics activity on silicate glasses in an experimental laboratory, which main interest is the study of the glass phase by the mean of spectroscopy techniques. The aim of this *ab initio* activity is to understand how the silica network is disrupted when modifier ions such as sodium or calcium are added to the system and to which extent the structural, dynamical and electronic properties can be affected.

Volker Heine was the initiator of my visit, and we had very useful and stimulating discussions about theoretical questions encountered in silica glass and minerals. In particular, one of our common interest lay in the network breaking and rebridging in silicate melts and the way this process leads to the glass formation. Another interesting question concerned the similarities between the structural and vibrational properties of the amorphous and some crystalline phases of silica: this could give rise to an interesting study in connection with the Rigid Unit Mode theory.

I also had the opportunity to visit three different departments: Theory of Condensed Matter in the Cavendish laboratory, the department of Earth Sciences and the department of Chemistry. In the three departments, I had very interesting discussions with specialists of glasses and minerals (Martin Dove, Steven Elliott, Ian Farnan ...) or specialists of *ab initio* simulations (Mike Payne, Carla Molteni, Ali Alavi, Michiel Sprik ...). In particular, the technical difficulties in generating a glass using *ab initio* molecular-dynamics simulation have been tackled and some ideas emerged in order to deal with the too fast quench rate, the small size of the system and the high energy cuttoff used in this kind of study.

During my visit, a round table was organized in order to discuss how computer simulations can help to understand the unsolved problems in glasses. The persons present at this round table were: V. Heine, M. Dove, S. Elliott, I. Farnan, post-docs and PhD students. Among others, the subject of the low frequency dynamics in glasses has been examined as well as some problems related to rheology and diffusion mechanisms in melts.

Overall my visit to Cambridge was very fruitful and I am very thankful to the Ψ_k network for making it possible.

Magali Benoit

Report on the collaborative visit of Stefano Fabris (Max-Planck-Institut Stuttgart) to Prof. Michael W. Finnis (Queen's University Belfast)

November 21-26, 2000

Tight-Binding modelling of alumina

I visited Prof. Michael W. Finnis and Dr Barbara Montanari (Queen's University Belfast) from the 21^{st} to the 26^{th} of November 2000. The purpose of my visit was to discuss recent achievements and future directions of our collaboration on tight-binding modelling of alumina (Al_2O_3).

Prof. Finnis and coworkers have recently shown how the structural and electronic properties of partial covalent oxides may be captured by including atomic polarisability in a self-consistent tight-binding scheme [Finnis *et al.*, Phys. Rev. Lett. **81**, 5149 (1998)]. The model was successfully applied to zirconia (ZrO_2) [Fabris, Paxton, Finnis, Phys. Rev. B **61**, 6617-6630, (2000); Phys. Rev. B, 63, to appear, (1 February 2001)]. We are now trying to apply it to alumina (Al_2O_3) as well.

During my stay, Dr Montanari and I have been working on the parameterisation of the tight-binding Hamiltonian by which we can now describe the electronic band structure of alumina. In particular, we discussed how to capture the unusual lattice parameter-dependence of the bandgap and bandwidths. Preliminary test showed that those effects could be captured with the inclusion of non-zero overlap matrix element S_{ij}, and atomic polarisability.

The visit gave me also the opportunity to discuss with Dr Tony Paxton the recent modifications of the computer code we use for the tight-binding calculations, and to review with Dr. Paxton and Prof. Finnis our future publications.

In conclusion the visit was very fruitful and I am grateful to the Ψ_k network for the financial support.

Stefano Fabris

6.3 Workshop/Conference Announcements

6.3.1 FHImd Hands-on Workshop

APPLICATION OF DENSITY-FUNCTIONAL THEORY IN CONDENSED MATTER PHYSICS, SURFACE PHYSICS, CHEMISTRY, ENGINEERING AND BIOLOGY

23 July - 1 August 2001, Berlin

http://www.fhi-berlin.mpg.de/th/Meetings/FHImd2001/

Sponsored by the Fritz-Haber-Institut der Max-Planck-Gesellschaft and the Psi-k Network

This hands-on course focuses on the application of density-functional theory to electronic-structure calculations in different scientific fields and provides a practical introduction to the handling of pertinent software packages. As a specific example we consider the computer code FHImd. The workshop programme combines morning lectures, which elucidate the theoretical concepts and numerical procedures, with practical sessions in the computer laboratory where realistic research problems are tackled. In addition to condensed matter physics, special emphasis is placed on nontraditional fields like biology and surface chemistry. The workshop is part of a biennial series and follows previous events in Berlin (1995, 1997) and Trieste (1999).

Applications for this workshop should be submitted until 31 March 2001. Further details and instructions how to apply are available at

http://www.fhi-berlin.mpg.de/th/Meetings/FHImd2001/

6.3.2 ESF/CECAM Workshop

Ab Initio Modelling in the Biological Sciences

Lyon, June 11-13, 2001
sponsored by the Psi-k/ESF Network and CECAM

This workshop will bring together researchers with experience in applying and developing ab initio quantum mechanical simulations with scientists working in biological- and life-sciences. The goal is to achieve a mutual understanding of the capabilities of ab initio modelling and the important biological problems to which they may be applied.

More details can be found on the web page at:

http://www.tcm.phy.cam.ac.uk/ mds21/Workshop2001/

Organisers:

Matthew Segall (mds21@phy.cam.ac.uk)
Ursula Roethlisberger (uro@inorg.chem.ethz.ch)
Paolo Carloni (carloni@sissa.it)

If you are interested in participating in this workshop, please contact one of the organisers with the title of your proposed submission. A limited number of bursaries will be available to subsidise participation by young researchers. Please indicate if you would like to apply for a bursary.

6.3.3 Workshop on Local Orbitals

Local orbitals and linear-scaling ab initio calculations

CECAM, Lyon, France

3–7 September 2001

`http://www.tcm.phy.cam.ac.uk/LocalOrbital/`

Aim

This workshop, jointly supported by CECAM and the ESF STRUC-Ψ_k Programme, aims to bring together scientists from a wide variety of communities who use local-orbital techniques for electronic structure calculations and atomistic simulations, with a particular emphasis on linear-scaling methods. This follows on from the successful workshop on localized orbitals held at CECAM in 1998.

Five sessions have been planned:

1. Atomic type orbitals
2. Gaussian type orbitals
3. Real space grid methods
4. Optimized orbitals
5. Linear-scaling methods

Invited speakers

Jerzy Bernolc, North Carolina State University, USA
Matt Challacombe, LANL, USA
Roberto Dovesi, Turin, Italy
Julian Gale, Imperial College, UK
Giulia Galli, LLNL, USA
Mike Gillan, University College London, UK

Stefan Goedecker, CEA Grenoble, France
Martin Head-Gordon, UC Berkeley, USA
Andrew Horsfield, Fujitsu ECIT, UK
Jürg Hutter, U. Zürich, Switzerland
Walter Kohn, UC Santa Barbara, USA
Richard Martin, UIUC, USA
Nicola Marzari, Princeton, USA
Pablo Ordejón, ICMAB-CSIC, Barcelona, Spain
Chris Pickard, Cambridge, UK
Gustavo Scuseria, Rice, USA
Gotthard Seifert, Paderborn, Germany
Uwe Stephan, Paderborn, Germany
Phil Sterne, LLNL, USA
David Vanderbilt, Rutgers, USA
Stan van Gisbergen, VU Amsterdam, The Netherlands
Mark van Schilfgaarde, Sandia, USA

Organizers

Peter Haynes
Theory of Condensed Matter
Cavendish Laboratory
Madingley Road
Cambridge CB3 0HE, UK

David Bowler
Department of Physics and Astronomy
University College
London WC1E 6BT, UK

Emilio Artacho
Dep. Física de la Materia Condensada
Universidad Autónoma de Madrid
C-III, 28049 Madrid, Spain

6.3.4 WideGap2001 Workshop

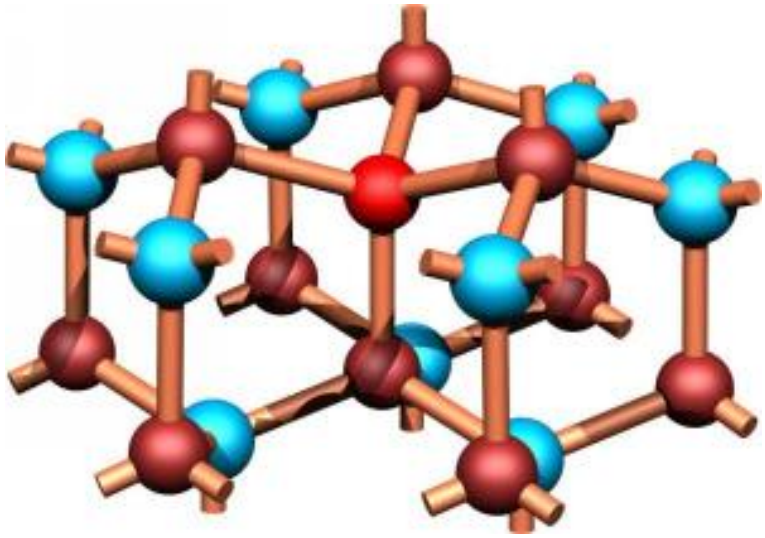
FINAL CALL FOR PAPERS

DOPING ISSUES IN WIDE BAND-GAP SEMICONDUCTORS

Exeter, United Kingdom, 21-23 March 2001

`http://newton.ex.ac.uk/widegap2001/`

Supported by the European Science Foundation through the Psi-k network.



Deadlines:	Please submit abstracts of your contributions by:	28 February 2001
	Early registration fee until:	28 February 2001

This is the final call for contributions. Please submit your abstract and register via the form provided on our web site: `http://newton.ex.ac.uk/widegap2001`.

Scope:

The aim of the workshop is to bring together experimentalists—interested in optimising and characterising the electrical activity of dopants in wide band-gap materials—and theoreticians who carry out calculations in this area. The workshop will focus mainly on defects and impurities in GaN, SiC, and diamond.

There is a great deal of interest in overcoming problems relating to shallow dopants in these materials. For example, boron is a shallow acceptor in diamond but there are problems relating to shallow donors. Phosphorus and sulphur are key candidates at the

moment and there is intense interest in optimising their activity.

In GaN, oxygen and silicon are known to be shallow donors but there are difficulties in finding efficient shallow p-type dopants - Mg and Be are favoured but have low activities. In SiC, nitrogen and boron on the Si site are the best donors available. Nevertheless all these dopants suffer problems relating to solubility and the formation of complexes.

Experimentalists are well aware that ab initio modelling is a very effective way in which dopant activity can be predicted. It is significant that the oxygen donor in GaN was first suggested from ab initio theoretical results.

There is current interest in co-doping where the electrical activity can be increased when two or more impurities (sometimes both donors and acceptors) are involved and this will be one of the topics at the workshop. Other topics will involve growth and characterisation.

This workshop will feature extended invited talks, contributed talks, and poster sessions. Ample time for informal discussions will also be provided. Proceedings will be published in a special issue of Journal of Physics: Condensed Matter. The workshop venue will be the campus of the University of Exeter, in the south-west of England. Accommodation will be provided on site in the University halls of residence.

Confirmed invited speakers include:

Friedhelm Bechstedt, Universität Jena, Germany
Bernard Clerjaud, Université Pierre et Marie Curie, Paris 6, France
Peter Deak, Budapest University of Technology, Hungary
Hiroshi Katayama-Yoshida, Osaka University, Japan
Christoph Nebel, Walter Schottky Institut, Garching, Germany
Joerg Neugebauer, Fritz-Haber-Institut, Berlin-Dahlem, Germany
Risto Nieminen, Helsinki University of Technology, Finland
Bo Monemar, Linköping University, Sweden
Juergen Ristein, University of Erlangen, Germany
John Robertson, University of Cambridge, UK
Bengt Svensson, Royal Institute of Technology, Stockholm, Sweden
Kimmo Saarinen, Helsinki University of Technology, Finland
Chris Van de Walle, Xerox PARC, Palo Alto, USA
Christian Wetzel, Uniroyal Optoelectronics, USA

Organisers:

R. Jones & C. J. Fall	Telephone: +44 1392 264134
School of Physics	Secretary: +44 1392 264151
University of Exeter	Fax: +44 1392 264111
Exeter EX4 4QL	Email: widegap2001@excc.ex.ac.uk
United Kingdom	

7 General Workshop/Conference Announcements

7.1 Enrico Fermi International School of Physics

HIGH-PRESSURE PHENOMENA

Varenna, Lago di Como, Italy
3-13 July 2001

High-pressure science is experiencing a surge of breakthroughs, with new discoveries resulting from a broad series of advances in experimental and theoretical techniques. "High-Pressure Phenomena" will be a one-of-a-kind Summer School that covers the breadth of the burgeoning, multidisciplinary field of high- pressure research – starting from experimental and theoretical fundamentals and extending to recent developments and applications in physics and chemistry, materials science and technology, Earth and planetary science, and biology.

DIRECTORS:

Guido L. Chiarotti - SISSA, Trieste
(guido@sissa.it)

Russell J. Hemley - Carnegie Institution, Washington, DC
(hemley@gl.ciw.edu)

SCIENTIFIC SECRETARIES:

Marco Bernasconi - University of Milano-Bicocca
(marco@mater.unimib.it)

Lorenzo Ulivi - CNR, Firenze
(ulivi@ieq.fi.cnr.it)

LECTURERS :

N. W. Ashcroft, R. Bini, R. Boehler, R. E. Cohen, G. Jenner, P. Loubeyre, J. Loveday H. K. Mao, P. F. McMillan, W. J. Nellis, M. Nicol J. P. Poirier, S. Scandolo, D. J. Stevenson,V. V. Struzhkin, K. Syassen, O. Tsiok, Y. Vohra, R. Winter, T. Yagi

Held at the prestigious and beautiful Enrico Fermi International School of Physics in

Varenna, Italy, the course will be run in a pedagogic style, as is customary for the School, with each of the instructors giving from 2 to 3 lectures. Additional talks by participants are also planned. The text of the lectures will be distributed at the School and then organized for publication in the series "Proceedings of the International School of Physics - Enrico Fermi".

TOPICS:

Experimental techniques:
diamond cells, large-volume presses, shock waves
Vibrational, electronic, and nuclear spectroscopy
Crystallography: neutron and x-ray
Elasticity, rheology, and transport properties
Condensed matter theory
Ab initio simulations
Low-Z molecular systems
Synthesis of new materials
Semiconductors, metals, and superconductors
High-pressure organic chemistry
Biological materials under pressure
Earth and planetary interiors

FOR FURTHER INFORMATION, INCLUDING POSSIBLE STUDENT SUPPORT CONTACT THE DIRECTORS OR SECRETARIES, OR VISIT

http://www.sif.it/sif/sif/varenna/

7.2 DFT Summer School

2nd Summer School on Computational Physics: Density Functional Theory
August 28 - September 1, 2001
Caramulo, Portugal

The Centre for Computational Physics (http://cfc.fis.uc.pt/) is organizing its 2nd Summer School on Computational Physics: Density Functional Theory. It will take place at Caramulo, a mountain resort in central Portugal, from August 28 - September 1. The school will start with some introductory lectures on Density Functional Theory, and will cover its computational aspects, modern developments, difficulties and future prospects. There will be both theoretical lectures and practical sessions.

The school webpage is at http://cfc.fis.uc.pt/events/DFT2001/.

Please forward this message to anyone you think might be interested.

Fernando Nogueira	Phone: + 351 239410622
Physics Department, University of Coimbra	Fax: + 351 239829158
3004-516 COIMBRA - PORTUGAL	email: fnog@teor.fis.uc.pt

7.3 Workshop at Princeton University

WORKSHOP ANNOUNCEMENT – FIRST CIRCULAR

"Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms"

Princeton University

15-18 June 2001

http://www.princeton.edu/ es2001

The Workshop on Recent Developments in Electronic Structure Algorithms is the 13th in the series of annual workshops that bring together active participants in electronic structure theory from universities, colleges, government labs, and industrial labs from around the world.

The invited presentations and contributed posters will describe new methods for computing previously inaccessible properties, breakthroughs in computational efficiency and accuracy, and novel applications of these approaches to the study of molecules, liquids, and solids.

More information about the workshop will become available at the workshop homepage http://www.princeton.edu/ es2001 ; the organizing committee can be contacted at es2001@princeton.edu.

8 General Job Announcements

Two Postdoctoral Positions in Condensed Matter Theory Lancaster University, Lancaster, United Kingdom

Condensed Matter Theory group at Lancaster University invites applications for two postdoctoral positions (RA) funded by the British Research Council.

1. One postdoctoral position is funded for up to 3 years, for working on the theory of kinetic and optical processes in carbon nanotubes. It is available starting from 15 March 2001. An expertise either in the quantum transport theory, or in the band structure calculations of carbon-based materials, or in the theory of excitons in semiconductors would be considered as an advantage.

2. The other position is funded for up to 2 years, for working on the theory of spin-polarised transport in hybrid nanostructures. It is available starting from 15 March 2001.

The Lancaster Condensed Matter Theory group currently includes Professors Vladimir I. Falko and C. Lambert, two Postdoctoral Fellows and eight PhD students working on various problems of mesoscopic physics and quantum transport in hybrid nano-structures. The group is the coordinating node of a European RTN and TMR network (see http://www.lancs.ac.uk/users/QDPCS) and has excellent computing facilities, including a large Beowulf-class computer. More information about the group can be found on our departmental web-sites:

http://www.lancs.ac.uk/users/spc/physics.htm
http://www.lancs.ac.uk/users/spc/conf/conf.htm

Applications (including CV, List of publications and names of 3 referees) should be sent to:

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

Fax: (44)-1524-844037
email: v.falko@lancaster.ac.uk

The deadline for applications is 21st February 2001.

P O S T - D O C T O R A L P O S I T I O N

Excited states in semiconductors: heterostructures and extended defects

Ohio State University

From March 2001 a postdoctoral position is available. Research focuses on quasiparticle energies of semiconductors. The projects will be developed with colleagues at Ohio State University, Bob Albers at Los Alamos National Laboratory and John Rehr at the University of Washington. Systems of high experimental or industrial interest will drive the research.

More details on the job and applying for it can be found at:

http://www.physics.ohio-state.edu/ wilkins/postdocjob-01.html

This URL has links to the activities of the group – currently containing two postdocs, four graduate students and two undergraduates. This hire would increase the postdocs to three; more graduate students are being recruited.

John Wilkins
Department of Physics
Ohio State University
174 W. 18th Avenue

P O S T - D O C T O R A L P O S I T I O N
Theory of Atomic and Molecular Manipulation
Chalmers/Göteborg University, Sweden

A post-doctoral position is available immediately in the group of Materials and Surface Theory to work on the theory of atomic and molecular manipulation under supervision of Professor Mats Persson. The successful applicant will work on the theoretical description and modeling of structures formed by and mechanisms underpinning manipulation of individual atoms and molecules with the scanning tunneling microscope in collaboration with the theory group and the experimental groups of the TMR network on "Atomic/Molecular Manipulation" (http://fy.chalmers.se/ap/TMR/) and the experimental group of Professor Wilson Ho, UCI, USA.

For some recent achievements, see, Physical Review Focus 6, Sep. 26 (2000) (http://focus.aps.org/v6/st14.html) on "Surfing in an atom's wake"; Phys. Rev. Lett. **85**, 2997 (2000) and Search and Discovery in Physics Today, February 2000 (http://www.aip.org/pt/feb00/scantun.htm) covering single molecule vibrational spectroscopy and microscopy.

Duration: The post is for 2-3 years and starting date will be as soon as possible.

Salary: For candidates with a PhD degree awarded no more than 2-4 years ago, we can offer a taxfree stipend in the range of about 25.000 - 30.000 euro/year.

Location: The work will be carried out in group of Material and Surface Theory (http://fy.chalmers.se/ap/msp/) in the Department of Applied Physics, School of Physics and Engineering Physics (http://www.fy.chalmers.se/) at Chalmers in the central part of Göteborg, Sweden

Qualifications: Candidates should have a PhD and a strong background in the theoretical and computational methods of condensed matter physics.

Application: Applicants should send a CV, a list of publications and names and phone numbers of a few referees to Mats Persson (address below). Please, note that this position is funded for the first year by the TMR program of the EU so only candidates from (non Swedish) European countries and associated members, that is, Iceland, Israel, Lichtenstein and Norway, can apply.

Prof. Mats Persson,
Department of Applied Physics,
Chalmers/Göteborg University,
S-412 96 Göteborg, SWEDEN
e-mail: tfymp@fy.chalmers.se
phone: +46-31-7723666
web page: http://fy.chalmers.se/ tfymp

Ph. D. or P o s t d o c t o r i a l P o s i t i o n

Technical University of Vienna, Austria

Institute for Physical and Theoretical Chemistry

A PhD or post-doctorial position funded by the Austrian Science Foundation is available in the area of

Electronic structure theory of highly correlated solids.

In our group we have developed the full-potential LAPW bandstructure package WIEN97 and in this project it is planned to apply the LDA+U and orbital- polarization methods within this code to correlated systems.

The position is available immediately.

She/he should have some experience in computational Condensed Matter Theory, Unix and Fortran programming is also of advantage.

Further information on our group can be found on:

http://www.tuwien.ac.at/theochem/

Applications with resumes, list of publications, and name (address) of referees should be sent to (preferably by email):

Dr. P.Blaha
Institut f"ur Physikalische und Theoretische Chemie
TU Wien
Getreidemarkt 9/156
A-1060 Vienna
Austria

E-mail: pblaha@theochem.tuwien.ac.at

D. Phil. Projects
Department of Earth Sciences
Oxford University, UK

There are a number of computational D. Phil projects among those offered by the Earth Sciences department at Oxford University. The main areas of interest are chemical reactions at mineral surfaces and high-pressure materials. Please see our website for more details. The list of potential projects may be found at the URL

http://www.earth.ox.ac.uk/Research/opports.html

This list is not exhaustive. Other sound project proposals within these areas of research will also be considered for studentships.

Dr Keith Refson
Department of Earth Sciences
Parks Road
Oxford OX1 3PR, UK
Keith.Refson@earth.ox.ac.uk
Tel: +(1865) 272026
Fax: +(1865) 272072

Post-Doctoral Position in Biological Computations

Massachusetts Institute of Technology
Department of Chemical Engineering

The Post-Doc will work with part of a group of experimentalists and molecular modelers to study reactions of proteins and the effects of solutes and solvents on these reactions. Research is targeted directly to areas of industrial interest.

The position is available immediately.

Applications with resumes, list of publications, and name (address) of referees should be sent by e-mail to:

Bernhardt Trout
Assistant Professor
Department of Chemical Engineering
Massachusetts Institute of Technology

Tel: (617) 258-5021
FAX: (617) 258-8224
email: trout@mit.edu
http://troutgroup.mit.edu

Mailing address:

77 Massachusetts Avenue, 66-556
Cambridge, MA 02139

Postdoctoral Position at Theoretical Division

Los Alamos, New Mexico 87545, USA

A postdoctoral position in theoretical studies of materials properties is available at the Condensed Matter and Statistical Physics Group, Theoretical Division, Los Alamos National Laboratory. The candidate should have enthusiasm/experience for the theoretical study of pursuing the understanding and predictions of materials properties using ab initio/atomistic methods. The position will be usually for 2 years and can be extended for the third year.

U. S. Citizenship is preferred but not required. Good publication records, undergraduate and graduate transcripts are desired. The candidate should have a Ph. D. in relevant fields granted within the last three years.

Please send the CV to :

S. P. Chen: sc@lanl.gov

or

S. P. Chen
T-11, MS-B262
LANL
Los Alamos, NM 87545, USA
fax: 505-665-4063
phone: 505-667-7346

POSTDOCTORAL RESEARCH ASSISTANT

First-principles simulation of oxide-aqueous solution interfaces

School of Physical Sciences, Canterbury, UK

Applications are invited for a three-year postdoctoral position to apply large-scale first-principles simulations to oxide- aqueous solution interfaces. This is a new and challenging field for first-principles research and one of great importance to many research areas. The goal of the project is to improve, or establish for the first time, the fundamental understanding of the following: surface hydroxylation and proton mobility; liquid structure and dynamics at the interface; the properties of adsorption complexes arising from small molecules in solution; and the dependence of all the foregoing on thermodynamic parameters. This is a chance to make major progress indescribing the interfacial properties that govern processes ranging from corrosion and weathering through to catalysis and sedimentation.

Informal enquiries to Philip Lindan, p.lindan@ukc.ac.uk.

Closing date for receipt of applications: 25 January 2001.

Position of Assistant-Doctorant at the EPF-Lausanne

The Institute for Numerical Research in the Physics of Materials (IRRMA) at the EPFL in Lausanne is seeking an outstanding PhD student to perform research in the domain of first-principles electronic structure calculations and quantum molecular dynamics simulations. The position, immediately available, requires a universitary degree in physics or physical chemistry (or equivalent), which should have been obtained by the starting date. The candidate will have teaching duties and shall prepare a doctoral thesis at EPFL. A good background in quantum mechanics and previous experience in FORTRAN programming are required. The interested candidates should send as soon as possible. their (1) curriculum vitae, (2) the list of passed examinations and relative marks, and (3) confidential letters of recommendation to

Dr. Alfredo Pasquarello,
IRRMA-EPFL,
PPH-Ecublens,
CH-1015 Lausanne,
Switzerland,
Tel. +41/21/6934416,
email: Alfredo.Pasquarello@epfl.ch.

More info on http://irrmawww.epfl.ch/ and

http://irrmawww.epfl.ch/ap/ap.html

Postdoctoral Researchers
National Microelectronics Research Centre (NMRC), Cork, Ireland

The Computational Modelling Group, NMRC is seeking Postdoctoral Researchers in the areas of chemistry, physics and engineering:

- molecular electronic transport/electronic structure theory
- modelling of endohedral fullerenes/nanotechnologies
- application of quantum chemistry to chemical vapor deposition growth

Well-qualified candidates will be considered for entry level tenure-track positions.

In addition, we are seeking PhD students who would like to visit the NMRC for a period of up to one year while continuing their PhD programmes at their home institute. Please see the advertisement below for Marie Curie Visiting Studentships.

NMRC is Ireland's largest research centre with a staff of over 200 and with extensive fabrication, characterisation and computational facilities. The NMRC is currently undergoing a phase of expansion under new Irish government initiatives in Information & Communication Technologies, Nanotechnologies and Biotechnologies.

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

Interested applicants may make informal queries to:

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

Telephone: +353 21 4904345
FAX: +353 21 4270271
WWW: http://www.nmrc.ie/research/compmodel

You can telephone NMRC Human Resources at +353-21-4904232. All enquiries and applications will be treated in the strictest confidence. Applicants should forward a detailed curriculum vitae to:

HR Department
NMRC, Lee Maltings, Prospect Row, Cork, Ireland.

Fax: +353-21-4904058, email: careers@nmrc.ie

Marie Curie Visiting PhD Student Fellowships

The Computational Modelling Group at the National Microelectronics Research Centre (NMRC), Ireland is seeking highly qualified doctoral candidates for extended visits of up to one year. The candidates will participate in NMRC research programmes while continuing the studies for the doctoral degree at their home institution. The Computational Modelling Group has activities and interests in most aspects of micro- electronics simulations: current active areas of research include materials, devices, process and packages. We are particularly interested in simulation activities that link different length and temporal scales. Topics of interest include but are not limited to quantum electronic transport, atomistic and/or ab initio process modelling, coupled thermal and electrical modelling, mesoscopic electronics and molecular electronics. Interested candidates are invited to send a curriculum vitae and the names and contact information for two references to the:

These positions will be held open until suitable candidates are found. EU residency requirements apply to these Marie Curie Fellowships. Further details of NMRC, Ireland may be found on the web site http://nmrc.ucc.ie

The NMRC is an equal opportunity employer.

9 Abstracts

Structural properties of lanthanide and actinide compounds within the planewave pseudopotential approach

Chris J. Pickard and Björn Winkler
Institut für Geowissenschaften, Universität Kiel,
Olshausenstr. 40 D-24098 Kiel, Germany
Roger K. Chen and M. C. Payne
TCM, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, UK
M. H. Lee and J. S. Lin
Departments of Physics and Chemistry, Tamkang University,
Tamsui, Taipei 251, Taiwan
J. A. White and V. Milman
Molecular Simulations Inc., 240/250 The Quorum, Cambridge, CB5 8RE, UK
David Vanderbilt
Department of Physics and Astronomy, Rutgers University,
New Jersey 08855-0849, USA

Abstract

We show that planewave ultrasoft pseudopotential methods readily extend to the calculation of the structural properties of lanthanide and actinide containing compounds. This is demonstrated through a series of calculations performed on UO, UO_2, UO_3, U_3O_8, UC_2, α-CeC_2, CeB_6, CeSe, CeO_2, NdB_6, TmOI, LaBi, $LaTiO_3$, YbO, and elemental Lu.

(Appeared in Phys, Rev. Lett., **85**, 5122-5125 (2000))
Reprints available from Chris J. Pickard: cjp20@phy.cam.ac.uk

Systematic prediction of crystal structures

Björn Winkler and Chris J. Pickard
Institut für Geowissenschaften - Universität Kiel,
Olshausenstr. 40, D-24098 Kiel, Germany
Victor Milman
MSI - Barnwell Road 240/250, The Quorum, Cambridge, UK
Georg Thimm
School of MPE - Nanyang Technology University, Singapore

Abstract

A generally applicable and systematic prediction of crystal structures and their properties has been an important goal of crystallography and materials science. Here we present such a general and systematic approach. This approach is based on a combination of graph theory with quantum mechanics. As an application, structures, properties and relative stabilities of small hypothetical carbon polymorphs with up to six atoms per unit cell are presented.

(To appear in Chemical Physics Letters)
Manuscripts available from: cjp20@phy.cam.ac.uk

Density functional study of charge disordering in $Cs_2Au(I)Au(III)Cl_6$ under pressure

Björn Winkler and Chris J. Pickard*
Institut für Geowissenschaften, Mineralogisch-Petrographisches Institut,
Christian Albrechts Universität,
Olshausenstr. 40, D-24098 Kiel, Germany
M.D. Segall
TCM Group, Cavendish Laboratory, Madingley Road,
Cambridge, CB3 0HE, United Kingdom Victor Milman
Molecular Simulations Inc., The Quorum, Barnwell Road,
Cambridge CB5 8RE, United Kingdom

Abstract

We demonstrate that density functional theory can be used to study the charge order/disorder transition in $Cs_2Au(I)Au(III)Cl_6$. The ground state structure of this mixed-valence compound is reproduced with satisfactory accuracy, and a discontinuous phase transition is calculated to occur at about 6-10 GPa, in agreement with published experimental values. The precision of the calculations and of previously published experiments is insufficient to unambiguously determine whether the transition is from I4/mmm to P4/mmm, or proceeds directly into a cubic phase with space group $Pm\bar{3}m$. Irrespective of the symmetry of the phase appearing at 6-10 GPa, the calculations show that the pressure-induced structural changes are accompanied by a charge disordering, and that all gold atoms are in the single-valence state, Au^{2+}, in the high pressure phase.

(Submitted to Phys. Rev. B)
Manuscripts available from: cjp20@phy.cam.ac.uk

* Present Address: TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

All-electron magnetic response with pseudopotentials: NMR chemical shifts

Chris J. Pickard*
Institut für Geowissenschaften, Universität Kiel,
Olshausenstrasse 40 D-24098 Kiel, Germany
Francesco Mauri
Laboratoire de Minéralogie-Cristallographie de Paris,
Université Pierre et Marie Curie,
4 Place Jussieu, 75252, 75252, Paris, Cedex 05, France

Abstract

A theory for the *ab initio* calculation of all-electron NMR chemical shifts in insulators using pseudopotentials is presented. It is formulated for both finite and infinitely periodic systems and is based on an extension to the Projector Augmented Wave approach of Blöchl [P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994)] and the method of Mauri *et al* [F. Mauri, B. G. Pfrommer, and S. G. Louie, Phys. Rev. Lett. **77**, 5300 (1996)]. The theory is successfully validated for molecules by comparison with a selection of quantum chemical results, and in periodic systems by comparison with plane-wave all-electron results for diamond.

(Submitted to Phys. Rev. B)
Manuscripts available from: cjp20@phy.cam.ac.uk

* Present Address: TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

First principles molecular dynamics simulations of pressure-induced structural transformations in silicon clusters

C. Molteni[1], R. Martoňák[2], and M. Parrinello[3]

[1] *Theory of Condensed Matter group, Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, UK*

[2] *Department of Physics, Faculty of Electrical Engineering, Slovak Technical University, Ilkovičova 3, 812 19 Bratislava, Slovakia*

[3] *Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

Abstract

Using a recently developed constant pressure *ab initio* molecular dynamics method for studying non-periodic systems, we have investigated pressure-induced structural transformations in silicon clusters. Pressure is applied and tuned through a liquid described by a classical potential, while the clusters are treated within a density functional theory scheme. Pressure-induced transformations in the $Si_{35}H_{36}$ and $Si_{71}H_{60}$ clusters show common characteristics, with a tendency towards metallicity at high pressure and a hysteretic behaviour when the pressure is released.

(J. Chem. Phys. in press)

Preprints available from: cm10020@phy.cam.ac.uk

Boron Nitride Polymers: new building blocks for organic electronic devices

Michel Côté, Peter D. Haynes and Carla Molteni
Theory of Condensed Matter group, Cavendish Laboratory, Cambridge, Madingley Road, Cambridge CB3 0HE, UK

Abstract

Modern electronic devices are increasingly being designed by combining materials with different electronic properties. The conventional semiconductor industry has achieved this by building heterostructures, such as quantum wells and superlattices, from materials with the same crystal structure but different constituent atoms. We propose that boron nitride polymers, with the same structure as organic polymers, will allow the same idea to be applied to polymer materials, already recognised as a cheap alternative to inorganic semiconductors. We demonstrate the similarity between organic polymers and their boron nitride analogues and then explore the potential innovations, including band gap tuning, that these new polymers could bring to organic polymer research.

(Phys. Rev. B, in press)
Preprints available from: cm10020@phy.cam.ac.uk

Ab initio elasticity and thermal equation of state of MgSiO3 perovskite

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

Abstract

We have used high-temperature ab initio molecular dynamics simulations to study the equation of state of orthorhombic MgSiO3 perovskite at lower mantle pressure-temperature conditions. We have determined the Gruneisen parameter, as a function of volume. Our state-of-the-art simulations, accurate to within 10on thermal expansion and Gruneisen parameter of MgSiO3 perovskite. The simulations were based on the generalised gradient approximation and pseudopotential plane wave scheme, and were performed using the VASP code. At ambient conditions we find the values of 1.86*10-5 K-1 and 1.51, for the thermal expansion and Gruneisen parameter, respectively, in excellent agreement with the latest experimental studies. Calculated elastic constants and static equation of state at 0 K agree well with previous simulations. We have found no evidence for the high-temperature phase transitions of orthorhombic of MgSiO3 perovskite to cubic or tetragonal phases at mantle temperatures.

(To appear in 'Earth and Planetary Science Letters, 2001, 184: 555-560)
Preprints available at http://slamdunk.geol.ucl.ac.uk/ artem
Contact person: A.R. Oganov (a.oganov@ucl.ac.uk)

Numerically improved computational scheme for the optical conductivity tensor in layered systems

A. Vernes[a)], L. Szunyogh[a,b)] and P. Weinberger[a)]

[a)] *Center for Computational Materials Science,*
Technical University Vienna,
Gumpendorferstr. 1a, 1060 Vienna, Austria
[b)] *Department of Theoretical Physics,*
Budapest University of Technology and Economics
Budafoki út 8, 1521 Budapest, Hungary

Abstract

The contour integration technique applied to calculate the optical conductivity tensor at finite temperatures in the case of layered systems within the framework of the spin–polarized relativistic screened Korringa–Kohn–Rostoker band structure method is improved from the computational point of view by applying the Gauss–Konrod quadrature for the integrals along the different parts of the contour and by designing a cumulative special points scheme for two–dimensional Brillouin zone integrals corresponding to cubic systems.

(Accepted to be published in J. Phys.: Cond. Mat.)
Postscript preprints are available from A. Vernes (`av@cms.tuwien.ac.at`)
or alternatively from `http://arXiv.org/abs/cond-mat/0012175`

Layer–resolved magneto–optical Kerr effect in semi–infinite inhomogeneous layered systems

A. Vernes [a)], L. Szunyogh [a,b)] and P. Weinberger [a)]

[a)] *Center for Computational Materials Science,*
Technical University Vienna,
Gumpendorferstr. 1a, 1060 Vienna, Austria
[b)] *Department of Theoretical Physics,*
Budapest University of Technology and Economics
Budafoki út 8, 1521 Budapest, Hungary

Abstract

The contour integration technique applied to calculate the optical conductivity tensor at finite temperatures in the case of inhomogeneous surface layered systems within the framework of the spin–polarized relativistic screened Korringa–Kohn–Rostoker band structure method is extended to arbitrary polarizations of the electric field. It is shown that besides the inter–band contribution, the contour integration technique also accounts for the intra-band contribution too. Introducing a layer–resolved complex Kerr angle, the importance of the first, non–magnetic buffer layer below the ferromagnetic surface on the magneto–optical Kerr effect in the Co | Pt_m multilayer system is shown. Increasing the thickness of the buffer Pt, the layer–resolved complex Kerr angles follow a linear dependence with respect to m only after nine Pt mono–layers.

(To be published in Phase Transitions)
Postscript preprints are available from A. Vernes (`av@cms.tuwien.ac.at`)
or alternatively from `http://arXiv.org/abs/cond-mat/0012176`

Structure and magnetism in thin films and multilayers of hexagonal ruthenium

D. Spišák, R. Lorenz and J. Hafner
Institut für Materialphysik, Universität Wien
A-1090 Wien, Austria

Abstract

The results of ab-initio calculations for the electronic structure and the magnetic moments of unsupported hexagonal thin Ru and Fe films, bulk Ru and Fe metals and Ru_5Fe_5 multilayer are presented with the focus on the crystallographic phase stability of the Fe layers. The calculated equilibrium lattice parameters of hcp Ru and Fe solids reproduce accurately the values found experimentally. For Ru/Fe multilayers it is demonstrated that in an Fe part of a multilayer an unusual hexagonal stacking with a distorted bcc-like local environment is more stable than the standard hexagonal close-packed stacking. The same result was obtained in thin Fe films and it is shown to be associated with band structure effects of Fe at the Fermi level. For thin films the ground state lattice parameters and magnetic states of films up to four monolayers were determined by total energy minimization. The faults in hexagonal planes stacking and interdiffusion do not lead to nonmagnetic Fe layers at the interfaces which were observed experimentally.

(Accepted for publication in Phys. Rev. B)
Contact person: D. Spišák (Daniel.Spisak@univie.ac.at)

Stability, electronic properties and chemical reactivity of palladium-vanadium (111) surface alloys

R. Hirschl[a], Y. Jeanvoine[b], G. Kresse[a] and J. Hafner[a]

[a] *Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria*

[b] *Université d'Evry-Val d'Essonne, Boulevard F. Mitterand, F-91025 Evry Cedex*

Abstract

We investigate the influence of vanadium impurities on the geometric and electronic properties of palladium (111) surfaces using density-functional calculations with Perdew-Wang general gradient approximations and PAW potentials. Single layer Vanadium concentrations ranging from $c_V = \frac{1}{9}$ to $c_V = 1$ in and under the Pd(111) surface are considered. The calculated supercells consist of four to six layer slabs separated by several layers of vacuum, allowing the uppermost layers to relax. The most favorable vanadium superstructure over a wide concentration range is $(\sqrt{3}\times\sqrt{3})R30°$. Adsorbed V atoms are only stable once they are incorporated into or under the Pd surface. An energy barrier of 0.7 eV for the exchange of an adsorbed V atom is determined by a nudged elastic band calculation. Vanadium impurities reduce the density of states of surface Palladium atoms at the Fermi level and shift their d-bands to lower energies which reduces adsorption energies. Our findings agree very well with experimental results.

(Accepted by Surface Science (ECOSS 19 proceedings)

Preprints available from: robin.hirschl@univie.ac.at

Phase diagram and electronic structure of Pd-V alloys: ab-initio density functional calculations

R. Hirschl[a], J. Hafner[a] and Y. Jeanvoine[b]

[a] *Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria*

[b] *Université d'Evry-Val d'Essonne, Boulevard F. Mitterand, F-91025 Evry Cedex*

Abstract

A parameter-free approach based on ab-initio density functional calculations is shown to describe phase stability and order-disorder transformations in Pd-V substitutional alloys and intermetallic compounds with remarkable accuracy, allowing first-principles calculations of the complete alloy phase diagram. The investigations are based on electronic-structure and total-energy calculations for ordered compounds and disordered alloys (treated in a supercell approximation) using gradient-corrected exchange-correlation functionals and a plane-wave based all-electron method. All calculations involve a complete optimisation of all structural degrees of freedom. The calculation of the free energies of the competing phases is based on rather simple mean-field descriptions of long- and short-range ordering phenomena, using concentration dependent interchange- and shell-interaction parameters. In addition, the electronic structures of ordered compounds and of substitutional alloys has been analysed.

(Submitted to J. Phys. Condens. Matt.)

Preprints available from: robin.hirschl@univie.ac.at

There is a true precurser for hydrogen adsorption after all: The system H_2/Pd(111) + subsurface V

M. Beutl, J. Lesnik and K. D. Rendulic
Institut für Festkörperphysik, Technische Universität Graz,
Petersgasse 16, A-8010 Graz, Austria
R. Hirschl, A. Eichler, G. Kresse and J. Hafner
Institut für Materialphysik and Center for Computational Materials Science,
Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

Abstract

The adsorption dynamics of H_2 on Pd(111) alloyed with V has been studied using molecular beam experiments (MB) and ab-initio density functional theory (DFT) calculations. The experiments show that dissociation on pure Pd(111) is dominated by dynamical steering and therefore shows strong rotational hindering. The alloy surface exhibits a sticking probability independent of rotational excitation and an isotropic distribution of inelastically scattered molecules, attributed to a dynamical precursor. DFT calculations of the potential energy surface and ab-initio simulations of scattering events demonstrates that the different behaviour of Pd and Pd/V surfaces arises from the existence of a flat physisorption state.

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Preprints available from: robin.hirschl@univie.ac.at

Locality properties and Wannier functions for interacting systems

Erik Koch
Max-Planck Institut für Festkörperforschung,
Heisenbergstraße 1, 70569 Stuttgart, Germany
Stefan Goedecker
Département de recherche fondamentale sur la matière condensée,
SP2M/NM, CEA-Grenoble, 38054 Grenoble cedex 9, France

Abstract

We define Wannier functions for interacting systems, and show that the results on the localization of the Wannier functions for non-interacting systems carry over to the Wannier functions for interacting systems. In addition we demonstrate that the characterization of metals and insulators by the decay properties of their respective density matrices does not only apply to non-interacting, but also to interacting systems. As a prototypical example of a correlated system we investigate the one-dimensional Hubbard model. We propose an expression for the density matrix of that model, and derive a relation between the decay constant of the density matrix and the gap.

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Latex-file available from E. Koch: `koch@and.mpi-stuttgart.mpg.de`

A novel multigrid method for electronic structure calculations

M. Heiskanen, T. Torsti, M. J. Puska, and R. M. Nieminen
Laboratory of Physics, Helsinki University of Technology,
P.O, Box 1100, FIN-02015 HUT, FINLAND

Abstract

A general real-space multigrid algorithm for the self-consistent solution of the Kohn-Sham equations appearing in the state-of-the-art electronic-structure calculations is described. The most important part of the method is the multigrid solver for the Schrödinger equation. Our choice is the Rayleigh quotient multigrid method (RQMG), which applies directly to the minimization of the Rayleigh quotient on the finest level. Very coarse correction grids can be used, because there is no need to be able to represent the states on the coarse levels. The RQMG method is generalized for the simultaneous solution of all the states of the system using a penalty functional to keep the states orthogonal. The performance of the scheme is demonstrated by applying it in a few molecular and solid-state systems described by nonlocal norm-conserving pseudopotentials.

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Manuscripts available from: Tuomas.Torsti@hut.fi

Adsorbate-induced demagnetization and restructuring of ultrathin magnetic films: CO chemisorbed on γ-Fe/Cu(100)

D. Spišák and J. Hafner
Institut für Materialphysik, Universität Wien
A-1090 Wien, Austria

Abstract

First-principles local-spin-density investigations of the structural, magnetic and electronic properties of clean and CO adsorbed ultrathin γ-iron films epitaxially grown on Cu(100) surfaces demonstrate that both the geometrical and the magnetic structures of the films are profoundly modified by the adsorption of CO. The enhanced magnetic moments of the top layer atoms are strongly quenched by the presence of the adsorbate. Due to the pronounced magnetovolume effect, this leads also to a correlated change in the interlayer relaxations. Strikingly, the adsorbate-induced demagnetization is primarily limited to those surface atoms directly bonded to the adsorbate. This leads to the formation of an in-plane magnetic pattern in a partially adsorbate-covered film. In addition, for the most stable solutions the vibrational eigenfrequencies of the CO adsorbate have been obtained.

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Contact person: D. Spišák (Daniel.Spisak@univie.ac.at)

Cd hyperfine fields at the bcc Fe/Co interface

V. Bellini, R. Zeller, P.H. Dederichs
Institut für Festkörperforschung, Forschungszentrum Jülich GmbH,
D-52425 Jülich, Germany

Abstract

We present *ab-initio* calculations for the magnetic properties of the (001) and (110) *bcc* Fe/Co interfaces. The calculations are performed by the Korringa-Kohn-Rostoker (KKR) Green's function method using the local density approximation of density functional theory. Of central interest is the relation between the hyperfine fields induced on substitutional Cd probe atoms and the magnetization profile at the interface. We compare the calculated Cd hyperfine fields with the ones measured by a time-differential Perturbed Angular Correlation (PAC) spectroscopic experiment [Swinnen *et al.*, Phys. Rev. Letters **78**, 362 (1997)]. The comparison suggests us that the considered interfaces between Fe and Co are strongly interdiffused, so that no "simplified" relation exists between the measured hyperfine fields and the magnetic moments at the interface.

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Manuscripts available from: Ru.Zeller@fz-juelich.de

Magnetic 4d monoatomic rows on Ag vicinal surfaces

V. Bellini, N. Papanikolaou, R. Zeller and P.H. Dederichs
Institut für Festkörperforschung, Forschungszentrum Jülich GmbH,
D-52425 Jülich, Germany

Abstract

The magnetic properties of $4d$ monoatomic rows on Ag substrates have been studied by *ab initio* calculations using the Screened Korringa-Kohn-Rostoker (SKKR) Green's Functions method within Density Functional Theory (DFT) in its Local Spin Density approximation (LSDA). The rows were placed at step edge (step decoration) and on terrace positions of different vicinal Ag surfaces, i.e. *fcc* (711), *fcc* (410) and *fcc* (221). The results for the magnetic moments are explained in terms of the different coordination number of the row atoms and the different hybridization between the rather extended $4d$ orbitals of the row atoms and the *sp*-like valence electrons of the Ag substrates. For the *fcc* (711) vicinal surface, we explore the possibility of antiferromagnetic coupling between the atoms in each row and discuss, by means of total energy calculations, the stability of the antiferromagnetic solutions with respect to the ferromagnetic ones.

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Manuscripts available from: Ru.Zeller@fz-juelich.de

Orbital Magnetism of Transition Metal Adatoms and Clusters on the Ag and Au(001) Surfaces

I. Cabria, B. Nonas, R. Zeller, P.H. Dederichs
Institut für Festkörperforschung, Forschungszentrum Jülich GmbH,
D-52425 Jülich, Germany

Abstract

We present ab-initio calculations of the orbital moments and magnetocrystalline anisotropy energies for 3d, 4d and 5d transition metal adatoms and for some selected small clusters on the (001) surfaces of Ag and Au. The calculations are based on the Local Density Approximation of Density Functional Theory and apply a fully relativistic KKR Green's function method. Due to the reduced coordination of the adatoms and the weak hybridization with the substrate, we find fairly large orbital moments, in particular for the elements towards the end of the series. The general trend can be understood from a simple tight-binding model. The orbital moments are connected with very large anisotropy energies. While the orbital moments are on the Ag substrate somewhat larger than on Au, the magnetic anisotropy has about the same size for both substrates. Calculations for small clusters of Fe, Ru and Os adatoms show, that due to interaction effects the orbital moments are strongly reduced, e.g., by 50 % for the dimer atoms. The size of the reduction correlates well with the coordination number. Similar reductions also occur for the magnetic anisotropy energies.

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Manuscripts available from: Ru.Zeller@fz-juelich.de

Quantum-well states mediated STM images of buried two-dimensional transition-metal alloys

D. Wortmann[†], S. Heinze[†,¶], G. Bihlmayer[†], and S. Blügel[†]
[†]*Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[¶] *Zentrum für Mikrostrukturforschung, Universität Hamburg, D-20355 Hamburg, Germany*

Abstract

We predict the possibility to image with the scanning tunneling microscope (STM) in the constant current mode interfaces of ordered alloys and compounds deeply buried below surfaces of metals with strongly dispersive electron states in the vicinity ($\sim \pm 1$ eV) of the Fermi energy. We report a theoretical study in which this assertion is verified for two-dimensional (2D) transition-metal alloy monolayers buried deeply below noble-metal surfaces. Employing the FLAPW method, first-principles calculations are performed for two systems: (i) Cu/p(2×1) CuIr/Cu(100), a 2D p(2×1) CuIr alloy, i.e. Ir chains, buried in Cu(100) and (ii) Ag/c(2×2) MnAg/Ag(100), a 2D c(2×2) MnAg alloy, i.e. a checkerboard arrangement of Mn and Ag atoms, buried in Ag(100). STM images and corrugation amplitudes were calculated using the Tersoff-Hamann model. Even after covering the ordered alloys with 11 layers of substrate atoms the calculated STM images display the pattern of the buried alloy layer. The corresponding corrugation amplitudes are above the experimental resolution limit. It is shown that the formation of quantum-well states between the buried alloy and the surface is the origin of this phenomenon.

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Copy available from: d.wortmann@fz-juelich.de

Surface Core Level Shifts of Clean and Oxygen Covered Ru(0001)

S. Lizzit, A. Baraldi, A. Groso
Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34012 Trieste, Italy
K. Reuter, M. V. Ganduglia-Pirovano, C. Stampfl, M. Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin-Dahlem, Germany
M. Stichler, C. Keller, W. Wurth, and D. Menzel
Physik-Department E20, Technische Universität München, 85748 Garching, Germany

Abstract

We have performed high resolution XPS experiments of the Ru(0001) surface, both clean and covered with well-defined amounts of oxygen up to 1 ML coverage. For the clean surface we detected two distinct components in the Ru $3d_{5/2}$ core level spectra, for which a definite assignment was made using the high resolution Angle-Scan Photoelectron Diffraction approach. For the $p(2 \times 2)$, $p(2 \times 1)$, (2×2)-3O and (1×1)-O oxygen structures we found Ru $3d_{5/2}$ core level peaks which are shifted up to 1 eV to higher binding energies. Very good agreement with density functional theory calculations of these Surface Core Level Shifts (SCLS) is reported. The overriding parameter for the resulting Ru SCLSs turns out to be the number of directly coordinated O atoms. Since the calculations permit the separation of initial and final state effects, our results give valuable information for the understanding of bonding and screening at the surface, otherwise not accessible in the measurement of the core level energies alone.

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Contact person: Karsten Reuter (reuter@fhi-berlin.mpg.de)

Oxygen Induced Rh $3d_{5/2}$ Surface Core-Level Shifts on Rh(111)

M. V. Ganduglia-Pirovano and M. Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin-Dahlem, Germany
A. Baraldi[1], S. Lizzit[1], G. Comelli[2,3], G. Paolucci[1] and R. Rosei[2,3]
[1]*Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34012 Basovizza, Trieste, Italy*
[2]*Dipartimento di Fisica, Università di Trieste, 34127 Trieste, Italy*
[3]*Laboratorio T.A.S.C.-I.N.F.M., S.S. 14 Km 163.5, 34012 Basovizza, Trieste, Italy*

Abstract

High resolution measurements are reported of the surface core-level shift (SCLS) of the $3d$ level for the Rh(111) surface as a function of oxygen coverage Θ on the surface. These measurements are analyzed by density-functional theory calculations of the initial- and final-state contributions to the shifts. The calculations are found to reproduce well the trends and magnitudes of the experimental shifts. Adsorption of oxygen shifts the Rh $3d$ surface core-levels to higher binding energies with the magnitude of the shift depending almost linearly on the coordination number of Rh surface atoms to O adatoms. The Rh $3d$ binding energy increases by about 0.3 eV per bond to an O adatom. This correlation is robust with respect to differencies between initial- and transition-state theory calculations of the SCLSs. The results are discussed in a simple physical picture.

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Contact person: M. Veronica Ganduglia-Pirovano (pirovano@fhi-berlin.mpg.de)

Assessment of exchange-correlation kernels for excited states in solids

Krzysztof Tatarczyk, Arno Schindlmayr and Matthias Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin-Dahlem, Germany

Abstract

The performance of several common approximations for the exchange-correlation kernel within time-dependent density-functional theory is tested for elementary excitations in the homogeneous electron gas. Although the adiabatic local-density approximation gives a reasonably good account of the plasmon dispersion, systematic errors are pointed out and traced to the neglect of the wavevector dependence. Kernels optimized for atoms are found to perform poorly in extended systems due to an incorrect behavior in the long-wavelength limit, leading to quantitative deviations that significantly exceed the experimental error bars for the plasmon dispersion in the alkali metals.

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Contact person: Krzysztof Tatarczyk (tatar@fhi-berlin.mpg.de)

Magnetic dichroism in electron spectroscopy

H. Ebert, J. Minár, and V. Popescu
Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 Munich, Germany

Abstract

A simple scheme that is based on the Green's function formalism is introduced, that allows to investigate spin-orbit-induced properties in magnetic solids in a very transparent way. This is demonstrated by investigations on the orbital magnetic moments, on the Fano effect in angle-integrated valence band photoemission and on magnetic circular dichroism in X-ray absorption. Numerical results obtained by additional fully relativistic calculations are presented to support the various conclusions drawn from the analytical considerations. This applies in particular to the interpretation of the magnetic circular dichroism in X-ray absorption (MCXD) on the basis of the so-called sum rules, which relate the dichroic spectra to the spin and orbital magnetic moments of the absorbing atom.

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Manuscript available as ps-file on request from
H. Ebert (Hubert.Ebert@cup.uni-muenchen.de)

Decomposition of the relativistic hyperfine interaction operator – with an application to the ferromagnetic alloy systems bcc-Fe_xNi_{1-x}, fcc-Fe_xPd_{1-x}, and fcc-Co_xPt_{1-x}

M. Battocletti and H. Ebert
Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 Munich, Germany

Abstract

A scheme developed by Pyper to decompose within relativistic Hartree-Fock theory the hyperfine interaction operator into the conventional Fermi contact, spin dipolar and orbital contributions is modified to split the hyperfine field of magnetic solids calculated in a fully relativistic way on the basis of spin density functional theory (SDFT) in an analogous way. The resulting expressions are used to examine the hyperfine fields for the disordered alloy systems bcc-Fe_xNi_{1-x}, fcc-Fe_xPd_{1-x}, and fcc-Co_xPt_{1-x} making use of the spin-polarized relativistic Korringa-Kohn-Rostoker Coherent Potential Approximation (SPR-KKR-CPA) method of band structure calculation. In particular the contribution of non-s-electrons to the hyperfine fields are discussed in detail. Special emphasize is laid on their relationship to the corresponding contributions to the spin and spin-orbit induced orbital magnetic moments.

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Manuscript available as ps-file on request from
H. Ebert (he@gaia.cup.uni-muenchen.de)

Microscopic origin of the magnetocrystalline anisotropy energy and van der Laan's conjecture in ferromagnetic-semiconductor multilayers

I. Cabria, A. Ya. Perlov, and H. Ebert
Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 Munich, Germany

Abstract

A study of the magnetocrystalline anisotropy energy (MAE) and orbital moment of ferromagnetic-semiconductor (FS) multilayers, bcc Fe/Ge (001) and bcc Fe/GaAs (001) alternating layers, is presented. The spin-orbit induced electronic MAE has been computed with the force theorem, using the ab initio spin-polarized relativistic (SPR) LMTO method and simulating the multilayers as superlattices. We have also computed the dipolar contribution to the MAE and the orbital moment of these multilayers. We have studied the stability of the electronic MAE respect to the number of k points and found stable MAE values. The electronic MAE is, in general, about two or more times larger than the dipolar MAE. The total MAE of these multilayers favours a perpendicular orientation of the magnetization respect to the plane of the layers and decreases, in general, (is more negative) when increasing the number of Fe layers. We have found that the interface Fe layer, in contact with the semiconductor layers, is the main responsible of the electronic MAE. We have verified in our calculations that the relationship between the electronic MAE and the orbital moment proposed by van der Laan, which states that the MAE is related with the spin sub-band orbital moments and not only with the total orbital moment, is very well satisfied in these systems. As far as we know, these are the first ab initio calculations which confirm the van der Laan's conjecture. Finally, analyzing the results by means of this conjecture we have arrived at the conclusion that the microscopic origin of the MAE of these multilayers is mainly due ($\sim$ 75 - 85 per cent) to the 3d spin down electrons of the interface Fe layers ($\sim$ seven electrons per unit cell) and that the source mechanism of the MAE is a delicate balance between the occupations of certain 3d spin down levels for different magnetization's directions.

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Manuscript available as ps-file on request from
H. Ebert (he@gaia.cup.uni-muenchen.de)

Relativistic calculation of magnetic linear response functions using the KKR-Green's function method

M. Deng, H. Freyer, J. Voitländer, and H. Ebert
Physikalische Chemie, Universität München,
Butenandtstr. 5-13, D-81377 Munich, Germany

Abstract

The relativistic KKR (Korringa-Kohn-Rostoker) Green's function method of band structure calculation supplies an extremely flexible basis to calculate magnetic linear response functions of solids. An important feature of this approach is that it accounts properly for the influence of all relativistic effects. A brief introduction to this formalism is presented together with some recent extensions to it. In particular, the inclusion of the orbital magnetization density induced by an external magnetic field allows a direct comparison with experiment for many different properties. This is demonstrated for the induced magnetic form factor, the magnetic susceptibility and the Knight shift of transition metals. A further appealing feature of the KKR-formalism is that it is applicable in principle to any complex system. This property is exemplified by applications for the disordered alloy systems Ag_xPd_{1-x} and Ag_xPt_{1-x} that are treated with the help of the Coherent Potential Approximation (CPA) alloy theory.

(Submitted to the Proceedings of the TMS2001 Conference)
Manuscript available as ps-file on request from
H. Ebert (he@gaia.cup.uni-muenchen.de)

10 Book Announcement

Superconductivity: Elementary Topics

by Prof. Keshav N. Shrivastava
School of Physics, University of Hyderabad, India

The elementary introduction to superconductivity along with hybridization of bands is given. The flux quantization is described along with the fractional flux as seen by resistivity. The flux-lattice and its melting has been discussed. Josephson effect and flux quantization are explained. Magnetization including para-Meissner effect and fractional flux has been described. The surface resistivity along with the London penetration depth and the effect of electric fields on the superconductors has been discussed. The microwave absorption in superconductors is given. The Moessbauer effect in superconductors is described. Levitation along with a measurement of mass of a superconductor as a function of distance from a magnet is explained. Fractal penetration of field in superconductors along with scaling exponents is given. NMR in superconductors along with the mixed-wave gap is described. There are appendices on superconducting compounds, the isotope effect, symmetries including s and d wave admixtures, time reversal invariance, pseudogap, relativistic effects including Cherenkov effect in Josephson junctions, soft vortices, specific heats and the quantum Hall effect. There is experimental data almost in every chapter. It is easy to read and may be used to teach a course. It is up to date and covers topics not given in other equivalent texts.

WORLD SCIENTIFIC Pub. Singapore, River Edge N.J. (U.S.A.), London, Hong Kong 2000. Office in Teipei, Taiwan, R.O.C., ISBN 981-02-4451-7.

The book may be purchased from:

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11 SCIENTIFIC HIGHLIGHT OF THE MONTH

Real-space relativistic spin-polarized photoemission

M. Woods[1], P. Strange[1], A. Ernst[2,3], and W. M. Temmerman[2]

[1]Department of Physics, Keele University, Staffordshire, ST5 5DY, England
[2]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England
[3]Max-Plank-Institut fur Mikrostukturphysik, Weinberg 2, D-06120 Halle, Germany

Introduction

It is now a routine matter to calculate band structures using the local density approximation (LDA) to Density Functional Theory (DFT). A full knowledge of the electronic structure is the key to understanding the solid state properties of a material. Experimentally, the probe of choice for determining the electronic structure on a band by band basis is angle-resolved photoemission spectroscopy (ARPES) [1]. The availability of a variable photon energy source in the form of synchrotron radiation has made angle-resolved photoemission into a practical and versatile tool in physics. Photoemission provides a convenient and much-used probe of the electronic properties [2]. The basis of this spectroscopy is the photoelectric effect in which the energy of an incident photon is transferred entirely to an electron of the irradiated material. If the energy of the incident photon is large enough for the electron to overcome the work function of the solid, the electron can escape the material and is detected by an electron spectrometer. In photoelectron spectroscopy the surface of the sample is irradiated by monochromatic light of energy $\hbar\omega$ and the kinetic energy of the emitted electrons is measured. Angle-resolved photoemission determines, as well as the energy, the emission angle of the photoelectrons and thus measures the external momentum. Finally, in spin- and angle-resolved photoemission the polarisation of the emitted electrons can also be analysed. These observables yield information about the binding energy E_B, the momentum $\mathbf{k}$, and the spin $\mathbf{s}$ of the electrons inside the solid. By proper choice of the angle and polarization of the incident radiation, the analysis of the obtained electron energy spectrum can be simplified enormously by the symmetry selection rules [3].

The need for a relativistic approach to the theory of photoemission is clear. Relativistic effects such as spin-orbit coupling, play a key role in the electronic structure of all materials, and this increases dramatically with atomic number. These effects were studied in pure metals by

McDonald *et al.* (1981) [4] and Fasol *et al.* (1988) [5] and in random alloys by Ginatempo and Staunton (1988) [6]. Strange (1998) [7] discusses relativistic effects in solids in general. All these calculations have their foundations in relativistic spin-density functional theory so any calculation that bridges the gap between first-principles energy bands and experimentally measured photoemission spectra is worthwhile.

For pure metals the framework for the required calculations of the photocurrent has already been developed. A quite general theory that includes ferromagnetic order on an equal footing with relativistic effects was put forward by Ackermann and Feder (1985a) [8]. A theory of energy-, angle- and spin-resolved photoemission spectroscopy of non-magnetic crystalline metals on the basis of relativistic quantum mechanics was written down first by Ginatempo *et al.* (1989) [9]. Here I present a derivation of the theory of relativistic spin-polarized photoemission based on the real-space Green's function method [10]. The real-space multiple scattering theory offers a fertile field of investigations of systems with arbitrary arrangements of atoms. It also has the advantage of a simple expression for the photocurrent in terms of site-off diagonal multiple scattering quantities and the site dependent matrix elements. This theory implements the real-space theory of Durham (1984) [11], within the framework of the one-step model of Pendry (1976) [2]. The formulation of the theory of photoemission discussed here builds on previous work. The underlying theory of photoemission is identical to that of Ebert and Schwitalla (1996)[12], however, their implementation was for bulk materials only. In the present formulation a real space implementation has been developed analogous to the non-relativistic theory of Ernst *et al.* (1998)[13]. This means that we can treat systems of low dimension, particularly surfaces and nanostructures easily.

Theory

The relativistic theory of photoemission is really an application of the first order Golden rule, giving the transition rate between the initial state $|i\rangle$ and the final state $|f\rangle$ due to a perturbation. For a single process this is

$$T = -\frac{2}{\hbar}\sum_f \int\int \psi_f^\dagger(\mathbf{r}) H'(\mathbf{r}) \mathrm{I}m\mathbf{G}^r(\mathbf{r},\mathbf{r}';\epsilon_i) H'^\dagger(\mathbf{r}) \psi_f(\mathbf{r}') d^3\mathbf{r}\; d^3\mathbf{r}' \tag{1}$$

where

$$H'(\mathbf{r}) = -ec\alpha\cdot\mathbf{A}(\mathbf{r}) \tag{2}$$

is the perturbation responsible for the transition and describes the electron-photon interaction. Here $\mathbf{G}^r(\mathbf{r},\mathbf{r}';\epsilon_i)$ is the retarded Green's function at energy ϵ, and ψ_f is the so called time reversed low-energy electron diffraction (LEED) state given by

$$\psi_f(\mathbf{r}) = \phi(\mathbf{r}) + \int \mathbf{G}^r(\mathbf{r},\mathbf{r}';\epsilon) V(\mathbf{r}')\phi(\mathbf{r}')\mathbf{dr}'. \tag{3}$$

which describes the final state of the electron. This equation follows from the asymptotic formula of the retarded Green's function. The retarded Green's function $\mathbf{G}^r(\mathbf{r},\mathbf{r}';\epsilon_i)$ in equation (1) can be calculated using the powerful technique of multiple-scattering theory. The crystal potential $V(\mathbf{r})$ is the total potential in the one-electron Dirac Hamiltonian taken to consist of an array of

non-overlapping muffin-tin potentials representing the lattice of atoms.

$$V(\mathbf{r}) = \sum_i v_i(\mathbf{r} - \mathbf{R}_i) \tag{4}$$

Accordingly we write the total potential as a sum over the lattice sites R_i where $v_i(\mathbf{r})$ is a muffin-tin potential at site i. Outside the muffin-tins a constant potential is assumed.

An essential feature of this approach is the use of the τ-matrix representation of multiple-scattering theory developed by Györffy and Stott [10] in which the retarded Green's function is defined as

$$G^r(\mathbf{r}, \mathbf{r}', \epsilon) = \sum_{\Lambda_1} \sum_{\Lambda_2} Z_{\Lambda_1}(\mathbf{r}; \epsilon) \tau^{ij}_{\Lambda_1 \Lambda_2}(\epsilon) Z^{\dagger}_{\Lambda_2}(\mathbf{r}'; \epsilon) - \sum_{\Lambda} Z_{\Lambda}(\mathbf{r}) J^{\dagger}_{\Lambda}(\mathbf{r}'; \epsilon) \;\; (r < r') \tag{5}$$

The τ-matrix $\tau^{ij}_{\Lambda'\Lambda''}(\epsilon)$, is a site and κm_j decomposition of the total T-matrix at energy ϵ and the $Z_{\Lambda'}(\mathbf{r}; \epsilon)$ and $J_{\Lambda'}(\mathbf{r}; \epsilon)$ functions are the regular and irregular solutions of the Kohn-Sham-Dirac equation with the single-site muffin-tin potential $v(\mathbf{r})$. These can be expanded in terms of radial and angular components:

$$Z_{\Lambda'}(\mathbf{r}; \epsilon) = \sum_{\kappa''=\kappa', -\kappa'-1} \begin{pmatrix} g^{m_j{}'}_{\kappa''\kappa'}(\mathbf{r}) \chi^{m_j{}'}_{\kappa''}(\hat{\mathbf{r}}) \\ i f^{m_j{}'}_{\kappa''\kappa'}(\mathbf{r}) \chi^{m_j{}'}_{-\kappa''}(\hat{\mathbf{r}}) \end{pmatrix} \tag{6}$$

and

$$J_{\Lambda}(\mathbf{r}; \epsilon) = \sum_{\kappa'=\kappa, -\kappa-1} \begin{pmatrix} g^{m_j \mathbf{i}}_{\kappa'\kappa}(\mathbf{r}) \chi^{m_j}_{\kappa'}(\hat{\mathbf{r}}) \\ \\ i f^{m_j \mathbf{i}}_{\kappa'\kappa}(\mathbf{r}) \chi^{m_j}_{-\kappa'}(\hat{\mathbf{r}}) \end{pmatrix}. \tag{7}$$

where the $\chi^{m_j}_{\kappa}$ are the usual relativistic spin-angular functions. Using equation (5) for the retarded Green's function with $r < r'$ in the Dyson equation (3) the time-reversed LEED state takes the following convenient form:

$$\psi_f(\mathbf{r}) = \frac{4\pi}{\sqrt{V}} \left(\frac{W + mc^2}{2W} \right)^{1/2} \sum_{\kappa m_j} (-i)^l C(l \tfrac{1}{2} j; m_j + m_s \; - m_s) Y_l^{m_j - m_s}(-\hat{k}) \sum_j e^{ik \cdot R_j} \sum_{\Lambda} \tau^{ij*}_{\Lambda'\Lambda}(\epsilon) \left[\hat{\tau} Z_{\Lambda'}(\mathbf{r}; \epsilon) \right] \tag{8}$$

where $C(l \frac{1}{2} j; m_j + m_s, -m_s)$ is a Clebsch-Gordon coefficient, $Y_l^{m_j + m_s}(-\hat{k})$ is a complex spherical harmonic, and $\hat{\tau}$ is the time-reversal operator. W is the total energy, including the rest mass energy. Equation (9) is the expression for the final state of the electron after photoemission.

Using the τ representation of the retarded Green's function (5) and equation (9) in (1), the photocurrent can be given as a sum of the inter-site contribution $M_{ij}(\epsilon + \hbar\omega)$, and the intra-site contribution $I_i(\epsilon + \hbar\omega)$:

$$T = \sum_{ij} M_{ij}(\epsilon + \hbar\omega) + \sum_i I_i(\epsilon + \hbar\omega). \tag{9}$$

The separation of the photocurrent equation into two contributing terms is done for convenience only because the intra-atomic term $I_i(\epsilon + \hbar\omega)$ vanishes for real energies and need not be calculated in this case. Thus we have obtained a fully relativistic photocurrent formula which is valid for any atomic arrangement. In essence we need to solve the multiple-scattering problem, that is

to find the single-site solution for the t-matrix, and the τ-matrices for low and high energies, which can be done using many well known methods.

One approach is the real-space cluster method for evaluating (5) and (9). In this case the τ-matrix can be obtained by inversion of the KKR matrix:

$$\underline{\tau}(\epsilon) = [\underline{t}^{-1}(\epsilon) - g_0(\epsilon)]^{-1} \tag{10}$$

For sufficient accuracy to describe real surfaces one usually needs to take into account a sufficiently large cluster. Our experience has been that we require at least about 100 atoms, because of the long range behaviour of the structure constants.

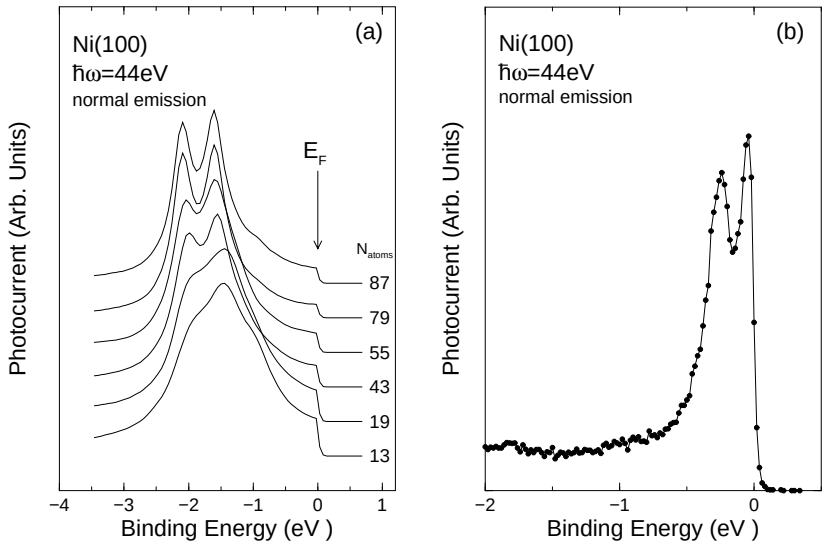

Figure 1: Photoemission spectrum of Ni(100). (a) Calculated photoemission spectra from different sized fcc configured clusters of atoms. (b) Experimental photoemission spectrum of Ni(100).

Figure 1 shows the convergence of the angle-resolved photocurrent for incident light of $\hbar\omega$=44.0 eV as a function of the size of cluster. Our calculations have been performed with broadening in the energy of 0.01 Ryd. What is evident is that the main features of the experiment (Figure 1(b)) are revealed by a relatively small cluster of 45 atoms but the Bloch State appears when the features no longer shift in energy ϵ which occurs with a cluster size of 87 atoms. The photocurrent for the cluster of 87 atoms is closer to the experiment but in this case the KKR-matrix is large, approximately 2800×2800, and needs 1.5 hours of CPU on a Dec Alpha 500 Series for the inversion of one energy point [14]. However with the inversion completed, the photocurrent for all θ and φ angles can be calculated without any further matrix inversion.

Calculations for Iron metal

Iron is an excellent metal to test relativistic theories because we have a reliable potential that reproduces experiment for Magnetic X-ray Circular Dichroism in absorption [15]. We have performed photoemission calculations on a cluster of 55 iron atoms where all atoms are described by identical bulk potentials. Clearly this takes into account surface geometry but neglects

changes in the potential due to the closeness of the surface. This is not a necessary restriction, but is done in this case for illustrative purposes only.

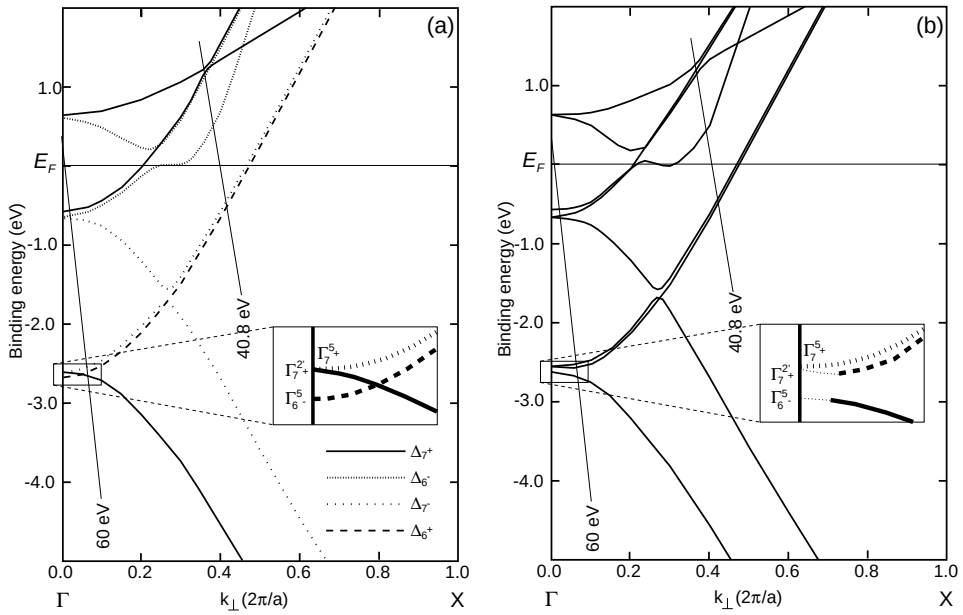

Figure 2: Symmetry resolved valence band structure of Fe(001). Bands with $\Delta_7+, \Delta_6+, \Delta_7-$ and Δ_6- double point group symmetry are distinguished as labelled in the figure. The thin solid lines are sections of the final state band, shifted down by the indicated photon energy. (b) as in (a) but for the Fe(100) direction.

Figure 2 shows the symmetry resolved band structure for Fe along two perpendicular directions of the Brillouin zone. Panel (a) shows the (001) direction with perpendicular magnetism. Panel (b) shows the (100) direction where the magnetic moment is oriented in plane. The (near) vertical solid lines are sections of the final state band shifted down by the energies used in the calculations. This clearly indicates the allowed transitions. At Γ the bands are identical in both figures of course. At Γ the band structure yields values for the exchange splitting of 2.1 eV and the crystal field splitting between the majority spin bands is 3.3 eV. The inset boxes in figure (1) not only show up the spin-orbit splitting at Γ but also clarify the differences in the band structure in the different directions as we proceed away from Γ. The differences in the bands are due to the subtle interplay between spin-orbit coupling and the magnetisation.

In figure (2) we observe the spin-resolved photoemission spectra attained with a 60 eV photon incident normal to the Fe(001) and Fe(100) surfaces. Incident radiation of this frequency probes the Brillouin zone close to Γ. Following Kuch *et al*[16] right and left circularly polarised incident photons will produce an asymmetry that is of use in determining the spin-orbit and magnetic anisotropy in local regions of k-space. Panel (a) decomposes the total photocurrent (solid line) generated with right circularly polarised photons into minority (dashed line) and majority (dotted line) spin contributions. Clearly the peak at -0.65 eV binding energy identifies transitions from the Δ_6^5+ band with a predominantly minority spin character. The peak at -2.5 eV marks transitions from the majority Δ_7^5- band. Panel (b) shows similar spectra attained with left circularly polarised incident radiation. This time the features mark transitions from Δ_6^5- at -2.6 eV and Δ_7^5+ at -0.55 eV. The total emission curves from panels (a) and (b) are brought

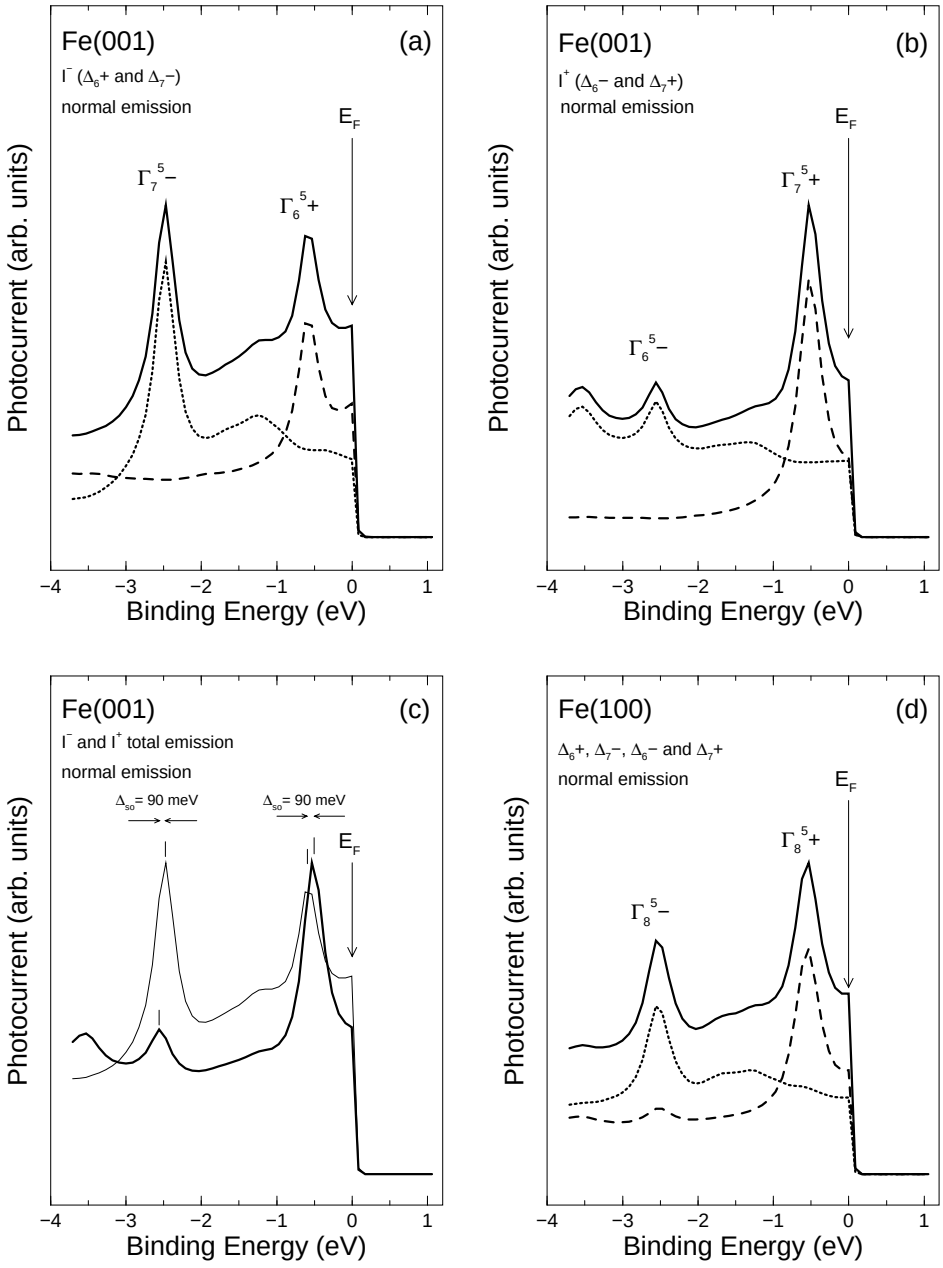

Figure 3: Spin-resolved photoemission spectra obtained with 60eV photons incident normal to the Fe(001) (perpendicular magnetisation) and Fe(100) (in-plane magnetisation). The calculations were performed with the same input parameters as used to calulcate the band structure of figure 2. Solid lines represent total emission and dashed (dotted) lines represent contributions from minority (majority) spin channels. (a) Right circularly polarised incident photons at the (001) surface. (b) Left circularly polarised photons incident at the (001) surface. (c) Assymetry between the totla spectra from panels (a) and (b) yielding the spin-orbit splitting. (d) Spin-resolved photoemission from the Fe(100) surface.

together in panel (c) and the spin-orbit splitting of 90 meV can be clearly seen.

We can compare the spectra probing close to Γ in both the (001) and (100) geometries. The in-plane magnetisation in the (100) case means there is no dichroism at normal incidence, the total photocurrent, and spin decomposed photocurrent for light incident normal to the Fe(100) surface is shown in panel (d). Comparison of the peak positions in panels (c) and (d) yields an energy shift of 50 meV. Similarly, at around -0.5 eV there is an energy difference of 50 meV due to the minority spin band with approximate Δ_6^5- symmetry shifting upwards and swapping places with the Δ_7^5- like band at Γ.

Figure (1) illustrates a common feature of band structures calculated relativistically, the avoided crossings at $k_\perp \approx 0.3(2\pi/a)$. At such points the bands may change their spin character, and consequently cannot be ascribed a spin label. Such points will yield common features in both the majority and minority spin photoemission spectra and identification of these points in the photoemission spectra with such band features should be straightforward.

Summary

We have reported on the development of a real-space fully-relativistic spin- and angle-resolved photoemission code in the independent particle approximation. The code takes potentials generated elsewhere and puts them into a geometry of choice. The method underlying this development is formulated in terms of multiple scattering theory with the real-space representation of the Green's function. The multiple scattering part in the photocurrent formula is separated from the angle-dependent part, leading to an essential simplification of the photocurrent calculations. The photocurrent formula is general and can be easily adapted to the symmetry of the problem at hand. The code is user friendly and yields results that can be used to give an easy handle on the main features of the photoemission spectra. The computations are limited by the size of the cluster that may be treated.

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