HCM Newsletter

Ψ_k Network

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

Number 13 February 1996

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Editorial

The **Editorial** is followed by the section **News from the Network**, where we have included the progress report, submitted to Brussels, on the Network activity in the past year.

In the section **News from the Working Groups** readers will find a report on a mini-workshop on "*Magnetic Nanostructures on Surfaces*" held last October in Jülich, and a report on a collaborative visit of M. Gillan and J. Holender (*University of Keele, UK*) to Vienna.

Then we enclose a first announcement of the Second Workshop on "**Full-Potential LAPW calculations with the WIEN95 code**" to be held in Vienna on April 9-13, 1996. Following this are: the second announcement of the **Bond Order Potential Workshop** in Oxford, and first announcements of the **Research Workshop on Condensed Matter Physics** in Trieste, 17 June-23 August, 1996, and of the European Conference on **Physics of Magnetism 96**, to be held in Poznan (Poland), June 24-28, 1996. Please note, that the Network funds cannot be used to pay for attending either the Trieste Workshop, Oxford Workshop or the Polish Conference, since these events are not organised by the Network.
Straight after these there are announcements of **Ph. D** positions in Halle and Exeter.

The **Abstracts** section is followed by the **Highlights of 1995** where we elaborate on some of the successful collaborations of the Network.

The *Network* has a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:
http://www.dl.ac.uk/TCSC/HCM/PSIK/main.html

This also contains pointers to several other nodes: *O.K. Andersen (Stuttgart)* which includes information on the **Network Conference**, *P. Blöchl (IBM, Zürich*, *M. Gillan (Keele)*, *E.K.U. Gross (Univ. Wurzburg)*, *B.L. Gyorffy (Bristol)*, *V. Heine (Univ. Cambridge)*, *J. Kübler (TH, Darmstadt)*, *R. Nieminen (TU, Helsinki)*, *J. Nørskov (TU, Lyngby)* with information on CAMP, *M. Scheffler (FHI Berlin)*, *K.-H. Schwarz (TU, Vienna)* and *A. Walker (UEA Norwich).* If you maintain a home page on your activities we will be happy to include a pointer from the *Network's* home page to your home page.

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

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

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

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News from the Network

In this section we enclose a progress report on the Network activity in 1995. This report, together with the highlights of Networks' collaborations, included in the last section of this Newsletter, has been forwarded to Brussels.

Progress Report
1 January 1995 - 31 December 1995

HCM ψ_k-Network on
Ab initio (from electronic structure) calculation of complex processes in materials

Contract Number: CHRXCT930369

Preamble

This network is characterized by a large number of nodes (40) and more than 200 participating researchers. The network aims to promote excellence in the subject of quantum mechanical calculations for electronic properties of solids through collaborations accross Europe including helping those in smaller, new or isolated research groups.

To operate efficiently as such a large network we have established a broadcast e-mail service and we publish a bimonthly newsletter which is e-mailed to over 250 researchers with network information on workshops, collaborations and scientific highlights. We run an abstract service through this newsletter and also through anonymous ftp and World Wide Web.

The stress which in 1994 was put on training and meetings, has this year resulted in 44 scientific publications. The full list of joint publications acknowledging the Network is included at the end of this report.

Factual Information

This year the Network has funded two Network Management Board Meetings at which current matters of running the Network and organisation of the Network Conference in September 1996 have been discussed and taken care of.

Two workshops and one mini-workshop have been organised this year. The workshop on "*Full Potential LAPW Calculations with the WIEN95 Code*" was a course where use of the latest electronic structure FP-LAPW WIEN95 code for solids was taught. Another workshop on "*Spin-Orbit Influenced Spectroscopies of Magnetic Solids*" was jointly organised with the ESF Network on "Relativistic Effects in Heavy Element Chemistry and Physics". Owing to that it was possible to bring together researchers (both theoreticians and experimentalists) from all over Europe, active in the topic of the Workshop, and related topics, to present and discuss their latest results and ideas. The mini-workshop was devoted to discussions and exchange of opinions on the subject of "*Magnetic Nanostructures on Surfaces*".

Well over twenty collaborative visits have taken place this year, ranging from joint development of computer codes, initiating new collaborative projects, to continuation of established collaborations. These have resulted in many scientific publications. Below we mention highlights of the established collaborations:

- A collaboration between M. Finnis (MPI-Metalforschung) and the group of V. Heine (University of Cambridge, UK) on interatomic forces (see refs. 9-10 in joint publication list).
- A collaboration between group of M. Scheffler (Fritz-Haber-Institut Berlin, Germany), and group of J. Hafner (Tech. Univ., Vienna, Austria) on adsorption of atoms at surfaces (see ref. 15 in joint publication list).
- A collaboration between J. Redinger (TU Vienna, Austria) and Stefan Blügel in Jülich (Germany) on surface magnetism (see ref. 33 in joint publication list).
- A collaboration between group of P. Weinberger (TU Vienna, Austria) and the group of P.H. Dederichs in Jülich (Germany) on the screened KKR (see ref. 41 in joint publication list).
- A collaboration between N. Stefanou (Univ. Athens, Greece) and the group of P. Dederichs in Jülich (Germany) on the electronic and magnetic impurities in solids (see refs. 29 and 30 in joint publication list).
- A collaboration between group of O.K. Andersen (MPI Stuttgart, Germany), group of W.M. Temmerman (Daresbury Laboratory, UK), and B.L. Gyorffy (Univ. Bristol, UK) on gap anisotropy of layered high temperature superconductors (see ref. 38 in joint publication list).
- A collaboration between H. Ebert (Univ. München) and G.Y. Guo (Daresbury Lab., UK) on relativistic spin-polarised spectroscopies (see ref. 16 in joint publication list).
- A collaboration between C. Koenig (Univ. Rennes) and P.Blöchl (IBM Zürich) on molecular materials (see ref. 18 in joint publication list).

- A collaboration between K.-H. Schwarz (TU, Vienna) and P.Blöchl (IBM Zürich) on zeolites (see refs. 42 and 43 in joint publication list).
- A collaboration between J.L. Martins (Portugal) and Van Camp and Van Doren (Belgium) on molecular dynamics of nitride materials.
- A collaboration between A. Svane (Univ. Aarhus, Denmark), H. Winter (Forschungszentrum Karlsruhe, Germany), and group of W. Temmerman (Daresbury Laboratory, UK) on self-interaction corrected LSD description of low carrier Kondo systems (Ce pnictides) (papers under preparation).
- A collaboration between group of J. Hafner (TU Vienna, Austria) and K.P. Bohnen (Forschungszentrum Karlsruhe, Germany) on ab-initio calculation of bulk- and surface-phonons for transition metals (publication in preparation).
- A collaboration between group of J. Hafner (TU Vienna, Austria) and group of M. Gillan (Univ. Keele, UK) on ab-initio calculations of the structural and electronic properties of molten chalcogenides.
- A collaboration between R. Perez (Madrid) and J. Payne (Cambridge) on first-principles simulation of nanoindentation on silicon surfaces (see ref. 32 in joint publication list).
- A collaboration between S. Crampin (Univ. Bath, UK) and J. Inglesfield (Univ. Nijmegen, The Netherlands) on embedding method for confined quantum systems and quantum well states (see ref. 8 and 40 in joint publication list).
- A collaboration between P. Weinberger (TU Vienna, Austria) and C. Sommers (Univ. Paris, Orsay, France) on interface exchange coupling (see ref. 37 in joint publication list).

Application of Funding

This year the Network has funded two Network Management Board Meetings, three workshops, over twenty secondements, and 28 visits to the three workshops. Please note, that secondments between Austria and Switzerland have been funded by the respective countries. Additionally, a sum of 4139 GBP has been transferred to fund a four months collaborative visit of R. Perez (Madrid) in the Cavendish Laboratory (University of Cambridge, UK)–starting from January 1, 1996, and a sum of 56120 GBP has been transferred to Max-Planck-Institute in Stuttgart for the Network Conference which is to be held in Schwäbisch Gmünd (Germany), 18-21 September, 1996. Moreover, the Network funds a half of the salary of the scientific secretary based in Daresbury Laboratory, UK.

Network's Management Board Meetings

Since this Network is such a large entity, in order to ensure its smooth activity, it is run by the Network Management Board (NMB). The latter consists of spokepersons of all the Working Groups and representatives of all the countries participating in this Network. The NMB meets every half a year.

- *4th Network Management Board's Meeting, University of Paris, 4th March, 1995.* Present: O.K. Andersen (*vice-chairman*, MPI Stuttgart), O. Bisi (Univ. Trento, Italy), P. Dederichs (IFF-KFA-Jülich, Germany), P.J. Durham (Daresbury Lab., UK), B.L. Gyorffy (Univ. Bristol, UK), J. Hafner (TU, Vienna, Austria), V. Heine (*chairman*, Cavendish Laboratory, UK), C. Koenig (Univ. Rennes, France), J.L. Martins (INESC Lisbon, Portugal), R. Nieminen (TU, Helsinki, Finland), J. Nørskov (TU, Lyngby, Denmark), C. Patterson (Univ. Trinity College Dublin, Ireland), Z. Szotek (*scientific secretary*, Daresbury Lab., UK), W. M. Temmerman (*coordinator*, Daresbury Lab., UK)

- *5th Network Management Board's Meeting, University of Paris, 28th October, 1995.* Present: O.K. Andersen (*vice-chairman*, MPI Stuttgart), O. Bisi (Univ. Trento, Italy), P. Dederichs (IFF-KFA-Jülich), M. Gillan (Univ. Keele, UK), B.L. Gyorffy (Univ. Bristol, UK), J. Hafner (TU, Vienna, Austria), V. Heine (*chairman*, Cavendish Laboratory, UK), J.E. Inglesfield (Univ. Nijmegen, The Netherlands), C. Koenig (Univ. Rennes, France), J.L. Martins (INESC Lisbon, Portugal), R. Nieminen (TU, Helsinki, Finland), J. Ortega (Univ. Madrid, Spain), C. Patterson (Trinity College, Dublin, Rep. of Ireland), M. Scheffler (Fritz-Haber-Institut Berlin, Germany), N. Stefanou (Univ. Athens, Greece), A. Svane (Univ. Aarhus, Denmark), Z. Szotek (*scientific secretary*, Daresbury Lab., UK), W. M. Temmerman (*coordinator*, Daresbury Lab., UK)

Teams

Coordinator: *W.M. Temmerman, Daresbury Laboratory, GB tel.: +44 1925 603227, fax: +44 1925 603634*

Other Participants:

O.K. Andersen, MPIF Stuttgart, DE (16 researchers)
A. Andriotis, FORTH, GR (6 researchers)
O. Bisi, Universita degli studi di Trento, IT (3 researchers)
P. Blöchl, IBM-Research Division, CH (2 researchers)
G. Boureau, Universite P.et M. Curie, FR (3 researchers)
J. Braun, Universitat Osnabruck, DE (4 researchers)
N. Christensen, Arhus Universitet, DK (2 researchers)
P. Dederichs, Forschungszentrum Julich, DE (10 researchers)
H. Ebert, Universitat Muenchen, DE (2 researchers)
M. Finnis, MPIM Stuttgart, DE (5 researchers)
F. Flores, Universidad Autonoma de Madrid, ES (7 researchers)
F. Gautier, Universite de Strasbourg, FR (6 researchers)
M. Gillan, University of Keele, GB (9 researchers)
S. Giuliano, Universita degli Studi di Messina, IT (4 researchers)
M. Gupta, Universite de Paris-Sud XI, FR (2 researchers)
B. Gyorffy, University of Bristol, GB (4 researchers)
J. Hafner, Technische Universitat Wien, AT (10 researchers)

V. Heine, University of Cambridge, GB (23 researchers)
J. Inglesfield, Katholieke Universiteit Nijmegen, NL (8 researchers)
P. Kelly, Nederlandse Philips Bedrijven BV, NL (4 researchers)
C. Koenig, Universite de Rennes I, FR (3 researchers)
J. Kübler, Technische Hochschule Darmstadt, DE (6 researchers)
F. Manghi, Universita degli studi di Modena, IT (6 researchers)
J. Martins, INESC Lisbon, PT (3 researchers)
R. Nieminen, Helsinki University of Technology, FI (10 researchers)
J. Norskov, Danmarks Tekniske Hojskole, DK (10 researchers)
C. Patterson, University of Dublin, IE (4 researchers)
J. Pollmann, Universitat Munster, DE (6 researchers)
H. Potatoglou, University of Thessaloniki, GR (6 researchers)
M. Scheffler, Fritz Haber Institut, DE (20 researchers)
K. Schwarz, Technische Universitat, Wien, Austria (4 researchers)
C. Sommers, Universite de Paris-Sud XI, FR (2 researchers)
M. Springborg, Universitat Konstanz, DE (1 researchers)
J. Staunton, University of Warwick, GB (5 researchers)
N. Stefanou, University of Athens, GR (2 researchers)
V. Van Doren, Universitair Centrum Antwerpen, BE (3 researchers)
A. Walker, University of East Anglia, GB (5 researchers)
P. Weinberger, Technische Universitat Wien, AT (11 researchers)
H. Winter, Kernforschungszentrum Karlsruhe, DE (3 researchers)

Collaborative Visits (Secondments)

Below we enumerate all collaborative visits that have taken place in 1995.

- **C. Sommers** (from *Univ. Paris Sud, Orsay* to *Technical University, Vienna, Austria*), 15th-19th January, 1995.
- **I. Mertig** (from *TU, Dresden, Germany* to *Technical University, Vienna, Austria*), 17-18th January, 1995.
- **J.E. Inglesfield** (from *Catholic University, Nijmegen* to *Technical University, Vienna, Austria*), 26-30th January, 1995.
- **M. Heinemann** (from *Catholic University, Nijmegen* to *Technical University, Vienna, Austria*), 26-30th January, 1995.
- **J. van Hoof** (from *Catholic University, Nijmegen* to *Technical University, Vienna, Austria*), 26-30th January, 1995.
- **S. Simak** (from *University of Rennes* to *MPI für Festkorperforschung, Stuttgart, Germany*), 6th-7th February, 1995.

- **K. Capelle** (from *Univ. Würzburg, Germany* to *Univ. Bristol, UK*), 24 February-4 March, 1995.
- **H. Ebert** (from *Univ. München, Germany* to *Daresbury Laboratory, UK*), 26-30 March, 1995.
- **P. Blöchl** (from *IBM Zürich* to *Technical University, Vienna, Austria*), 12 May-18 June, 1995.
- **A. Liechtenstein** (from *MPI für Festkorperforschung, Stuttgart* to *Univ. Oxford, UK*), 19-23 June, 1995.
- **H.M. Polatoglou** (from *Univ. Thessaloniki, Greece* to *MPI für Metalforschung, Stuttgart*), 24-26st May, 1995.
- **M. Deng** (from *Univ. München, Germany* to *Daresbury Laboratory, UK*), 17-30 June, 1995.
- **M. Rohlfing** (from *Univ. Münster, Germany* to *Cambridge Univ., UK*), 24 June-10 July, 1995.
- **A. Svane** (from *Univ. Aarhus, Denmark* to *Daresbury Laboratory, UK*), 25June-15 July, 1995.
- **H. Winter** (from *Forschungszentrum, Karlsruhe, Germany* to *Daresbury Laboratory, UK*), 23June-7 July, 1995.
- **M. Lüders** (from *Univ. Würzburg, Germany* to *Tech.Univ. Vienna, Austria*), 26 June-16 July, 1995.
- **J. Thijssen** (from *Catholic University, Nijmegen* to *Univ. Cambridge, UK*), 7-9th August, 1995.
- **A. Settles** (from *IFF,KFA-Jülich* to *Univ. München, Germany*), 6-10th August, 1995.
- **P. Ballone** (from *MPI für Metalforschung, Stuttgart* to *Univ. Cambridge, UK*), 21-25 October, 1995
- **C.M.J. Wijers** (from *Univ. Twente, The Netherlands* to *Univ. Aarhus, Denmark*), 2 November, 1995.
- **C. Katan (Hoerner)** (from *Univ. Rennes, France* to *IBM Zürich, Switzerland*), 5-18 November, 1995.
- **M. Gillan** (from *Univ. Keele, UK* to *Tech.Univ. Vienna, Austria*), 21-23 November, 1995.
- **J. Holender** (from *Univ. Keele, UK* to *Tech.Univ. Vienna, Austria*), 21-23 November, 1995.
- **C. Katan (Hoerner)** (from *Univ. Rennes, France* to *IBM Zürich, Switzerland*), 3-16 December, 1995.

- **E. Nusterer** (from *Tech.Univ. Vienna, Austria* to *IBM Zürich, Switzerland*), several extended visit totaling almost half a year.

Workshops

- **Full-Potential LAPW calculations with the WIEN95 code:** Vienna 19-22 April 1995
  The scientific programme of this workshop covered a short introduction to Density Functional Theory, band structure methods in general and the LAPW method, with corresponding algorithms in particular. The outline and handling of the new user-friendly program was described in detail, and the participants had also an opportunity to run the WIEN95 code on several workstations in five exercise sessions. Additionally, one day of the workshop was devoted to calculation of forces. Below we include the list of Network funded participants.

Participant	Node	Participant	Node
P. Alippi	Berlin	G. Botton	Cambridge
M. Fähnle	Stuttgart	B. Kohler	Berlin
H. Krimmel	Stuttgart	G. Nunes	Lisbon
S. Quassowski	Berlin	A. Rodriguez-Marco	Madrid

- **Spin-Orbit Influenced Spectroscopies of Magnetic Solids:** Herrsching 20-23 April 1995
  The European research in this field is very strong and this meeting brought together the leading European researchers. The papers presented at this Workshop are to be published in *"Lecture Notes in Physics"* (Springer-Verlag, 1996) (see ref. 44 in the list of joint publications). List of participants funded by the Network follows.

Participant	Node	Participant	Node
M. Battocletti	München	J. Braun	Osnabrück
K. Capelle	Stuttgart	P.H. Dederichs	Jülich
M. Deng	München	H. Demangeat	Strasbourg
H. Ebert	München	G.Y. Guo	Daresbury
B.L. Gyorffy	Bristol	J. Kübler	Darmstadt
P. Oppeneer	Darmstadt	J. Schwitalla	München
Z. Szotek	Daresbury	W.M. Temmerman	Daresbury
A. Vernes	München		

- **Magnetic Nanostructures on Surfaces:** Jülich 9-10 October 1995
  The purpose of this mini-workshop was to discuss and exchange expertise and ideas in the field and continue further development on the ab-initio KKR-GF technique. Also better ways of constructing potentials for more empirical schemes as EAM and EM were

discussed. List of participants is included below.

Participant	Node	Participant	Node
W. Hergert	Halle	V. Stepanyuk	Halle
C. Massobrio	Strasbourg	R. Zeller	Jülich
P.H. Dederichs	Jülich		

Joint Publications in 1995

This year the following 44 papers have been published or submitted for publication.

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[1] M. Biagini, C. Calandra, S. Ossicini, "Hole Filling and Interlayer Coupling in $YBa_2Cu_3O_7/PrBa_2Cu_3O_7$ Superlattices", Europhysics Letter **31**, 317-322 (1995).

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Newsletters

Moreover, the Network has published 6 Newsletters of both scientific and informative content. They were published in all even months of the past calendar year. These Newsletters are attached to this progress report.

News from the Working Groups

Report on the collaborative visit of M.J. Gillan and J. Holender (Univ. Keele, UK) to Vienna

21–23 November, 1995

Keele–Vienna Collaboration:

The Dynamical Simulation of Liquid Semi-Metals

M. J. Gillan$^\odot$, J. Hafner$^\oplus$, J. Holender$^\odot$, G. Kresse$^\oplus$ and F. Kirchhoff$^\odot$

$^\odot$ *Physics Department, Keele University,*
Staffordshire ST5 5BG, U.K.
$^\oplus$*Institut für Theoretische Physik, Technische Universität Wien,*
A-1040 Wien, Austria

The groups of Mike Gillan (Keele University) and Jürgen Hafner (Technische Universität, Wien) have started a collaboration on the first-principles simulation of liquid semi-metals, and specifically liquid Se and Te. Support from the network enabled Mike Gillan and Janusz Holender to make a short visit to Vienna in November last year to initiate this collaboration.

The collaboration is a very natural one, because the two groups have both been very active in first-principles molecular dynamics, and both have a strong interest in the simulation of metallic systems. Jürgen Hafner's interest in liquid metals and their alloys goes back many years [1]. Mike Gillan's interest is more recent, and started originally from his work on defects in crystalline metals [2]. Both groups have paid particular attention to the technical problems of doing robust and stable dynamical first-principles simulations on metallic systems [2-10]. A very positive aspect of the collaboration is that the two groups are working with two independent codes: the Keele group are using the Cambridge code CASTEP (or CETEP [11] on parallel machines), whereas the Vienna group are using their own code VAMP [12] (Vienna *ab-initio* molecular-dynamics package).

There are several reasons for studying the liquid chalcogens, but perhaps the most important is just sheer curiosity. Under ambient pressures, crystalline Se and Te consist of infinite chains, and are semiconducting ($E_g = 2.0$ eV) and semi-metallic respectively. The chain-like structure of Se survives into the liquid state, and so does its semiconducting character. This structure makes it highly viscous just above the melting point (490 K), though its viscosity drops quite rapidly to rather normal values on heating. In spite of this, the 2-fold average coordination is maintained up to at least 1770 K and 800 bar, and the three-dimensional structure of the liquid under these conditions is still highly controversial. Te is rather different, because its conductivity increases markedly on melting, and diffraction studies show that its first-neighbour coordination number increases from 2 to ~ 3. The structure of this liquid is still poorly understood.

Another reason for studying these systems is that they both pose a challenge to the local density approximation (LDA). This is clear already from calculations on c-Se by Hafner's group [13] and others. With the LDA, the equilibrium a lattice parameter comes out some 10 % too small. Problems with these materials are not too surprising, because there are both strong covalent bonds (responsible for the chain structure) and weak bonds (between the chains), and this is a good recipe for trouble. In fact, generalised gradient corrections put these solid-state problems right to a large extent for c-Se [13].

However, there is more trouble. Unpublished simulations of ℓ-Te by Florian Kirchhoff [14] done in Lausanne before he joined the Keele group showed a very serious disagreement with experimental results for the radial distribution function, with a first coordination number of about 6, instead of about 3. Completely independent simulations by the Vienna group have confirmed that there is a serious problem. Strangely, the problems seem to be less serious in ℓ-Se [15], even though there are definitely weak and strong bonds in the liquid. Again, the two groups have done completely independent calculations, which are in very satisfactory agreement with each other.

This collaboration promises to be extremely fruitful, and the discussions we had in November have got it off to a good start. The two groups are currently completing a set of simulations on ℓ-Se and ℓ-Te performed with the two codes, and we plan to write a joint paper in the near future. Apart from the scientific aspects, the groups have also found it very useful to compare in detail the techniques used in the codes, and we believe that in due course these comparisons will also prove helpful to the wider community.

References

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Report on the Miniworkshop
"Magnetic Nanostructures on Surfaces"
Jülich, Oct. 9 - Oct. 10, 1995

Participants: W. Hergert (*University Halle, Germany*)
V. Stepanyuk (*MPI Halle, Germany*)
C. Massobrio (*CNRS, University Strasbourg, France*)
R. Zeller (*Jülich, Germany*)
P.H. Dederichs (*Jülich, Germany*)

Two seminars were given on Oct. 9:

W. Hergert:	Ab-initio calculations of 3d transition metal (TM) clusters on Cu(001)
C. Massobrio:	Small copper clusters - a first principle approach

The first talk reported new results for the magnetic properties of small 3d-TM clusters on the Cu(001) surface. The calculations are done with a KKR-GF-method. The results are compared with the properties of 4d-TM on Ag(001), a different noble metal surface, previously studied by the Jülich group.

The second talk reported calculations for free Cu clusters ($n = 3 \ldots 9$). The calculations are done with a Car-Parrinello scheme using ultrasoft pseudopotentials (Vanderbilt). The properties of the Cu-clusters are compared with the results known for alkali-metal clusters. The results of the calculations of Cu-clusters compare very well with photoelectron experiments, performed in Prof. Eberhardt's group in Jülich.

Summary of the discussions during the miniworkshop

The discussions during the two days included two complexes:

1. Further developments of the ab-initio KKR-GF approach. Up to now the KKR-GF-programs are designed for the calculation of electronic and magnetic properties of small clusters on the ideal surface. Experimental investigations (in Kirschner's group, MPI Halle, STM investigations Fe/Cu(111)) show the importance of steps on the surfaces during the aggregation processes on the surface. Different possibilities are discussed to extend the KKR-GF-approach to steps on surfaces. This extension of the calculational scheme would allow also investigations of the properties of magnetic chains of atoms and clusters near steps on the surface.

2. Complementary information to ab-initio electronic structure calculations can be gained from MD simulations. Ab-initio calculations for large scale problems at surfaces are not possible up to now. Therefore more empirical schemes like (EAM, EM) are used to simulate surfaces processes. The results are not every time very satisfactory. We discussed to some extend the theoretical basis of these methods and different ways to improve these schemes by inclusion of either a better theoretical basis or the inclusion of surface properties in the construction of the interaction potentials.

W. Hergert

SECOND WORKSHOP

Full-Potential LAPW calculations with the WIEN95 code

April 9-13, 1996
Technical University Vienna, Austria
Chairman: K.Schwarz (TU-Vienna)
Email: kschwarz@email.tuwien.ac.at

First Announcement

Scope

This second workshop is concerned with recent progress in density functional calculations using the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the WIEN95 code (or related topics).

The workshop will be divided into two parts:

Part I: Introduction to WIEN95 (April 10-11)

- The LAPW method and the use of WIEN95 (an introduction)
- Hands on calculations with the new user-friendly code

Part II: Applications using the WIEN95 code mainly for experienced users (April 12-13)

- Results obtained with WIEN95 (including contributions by participants)
- Hands-on calculations with WIEN95
- Poster session

General Information

Conference site: The conference will take place at the Technical University in Vienna, A-1040 Vienna, Wiedner Hauptstr. 8-10, second floor (yellow tower, lecture hall 7)

World Wide Web homepage: http://www.tuwien.ac.at/theochem/
for continually updated information on the workshop.

Arrival: The workshop will start at 9 am on Tuesday (Thursday) for part I (II). Thus it is advised to arrive on April 9 (April 11, for part II).

Fee:		
	part I+II	2500 AS
	part II only	1000 AS
	accompanying persons	600 AS

Accomodation: The workshop starts directly after the Easter holidays. Therefore it is highly recommended to make hotel reservations as soon as possible.

MAKE YOUR OWN RESERVATION!

Below is a list of a few recommended hotels/accomodations with the prices quoted in Austrian Schillings per night and person.

Hotel	Address	Telephone	Price
Pensionhotel Schneider	A-1060 Vienna Getreidemarkt 5	+43-1-58838-0 +43-1-58838-212(Fax)	900
Hotel Attache	A-1040 Vienna Wiedner Hauptstr.71	+43-1-5051817 +43-1-5051817-232 (Fax)	600
Lehrerheim des Lehrervereins	A-1080 Vienna Langegasse 20-22	+43-1-403 23 580	350
Pension Felicitas	A-1080 Vienna Josefsgasse 7	+43-1-405 72 12	350
Youth Hostel	A-1070 Vienna Myrthengasse 7	+43-1-523 63 16 +43-1-523 58 49 (Fax)	50

For further addresses contact the organizer.

Please register soon!

Participants are encouraged to submit contributions in the form of talks (posters).

Deadlines: **Please register (see below) and pay before 15th March 1996**

Prof. K. Schwarz
Technical University Vienna
Getreidemarkt 9/158
A-1060 Vienna Austria
Email: kschwarz@email.tuwien.ac.at
Fax: +43 (1) 5868 937

Name and first name:
Professional title:
Address:
Phone:
Fax:
Email:
I wish to attend in part I (April 10-11) yes/no
I wish to attend in part II (April 12-13) yes/no
Please send me further information ( )
I plan to offer a contribution ( )
prefer poster ( ) or oral ( )
Tentative title ....
....
I will be accompanied by .... persons.
I am member of the HCM network (psik) yes/no
Date and Signature

2d Announcement

BOND ORDER POTENTIAL WORKSHOP

18 - 19 March 1996

UNIVERSITY OF OXFORD, DEPARTMENT OF MATERIALS
MATERIALS MODELLING LABORATORY

(Support from the EPSRC (U.K.) and the Naval Research Laboratory (U.S.A.) for travel and local expenses)

The realistic atomistic simulation of materials requires the quantum mechanical description of electron dynamics. Even with the highly efficient tight-binding (TB) model the $O(N^3)$ time scaling for matrix diagonalisation is crippling, and so linear O(N) methods are being developed for finding the total energy and forces on atoms.

During the first day of this two day workshop the background theory and concepts behind the novel Bond Order Potentials (BOPs) will be presented. BOPs provide an exact rapidly convergent many-atom expansion for the energy of a given bond within the tight-binding description of the electronic structure. Other important O(N) methods such as a density matrix method will also be described and their relative merits discussed with reference to particular modelling problems.

During the second day there will be an opportunity to learn about, and gain hands-on experience of the Oxford O(N) (OXON) modelling package. It will be distributed to all those interested in obtaining a copy.

PROGRAMME

MONDAY, March 18th, 1996

09:00–09:30	Registration	
09:30–11:00	Introduction: Tight-Binding and moments	D.G. Pettifor
11:00–11:30	Coffe	
11:30–12:30	The Bond Order Potentials method	A.M. Bratkovsky
12:30–14:00	Lunch	
14:00–15:00	The Density Matrix Method	A.P. Horsfield
15:00–15:45	Parallel BOP program and BOP applications	M. Fearn
15:45–16.15	Tea	
16:15–17:00	Comparisons of O(N) methods	D.R. Bowler
19:00	Dinner	

TUESDAY, March 19th, 1996

09:30–11:00	Hands-on session
11:00–11:30	Coffee
11:30–12:30	Hands-on session
12:30–14:00	Lunch
14:00–15:45	Pick up OXON computer package
15:45–16:15	Tea

- Anyone interested in attending should fill in the attached registration form and RETURN it to Dr Alex Bratkovsky by February 9th, 1996.
- The workshop expenses are:

Registration fee	none
Accommodation (Sunday-Monday nights)	34.50 GBP
Breakfast (Monday and Tuesday)	7.30 GBP
Lunch (Monday and Tuesday)	12.80 GBP
Dinner (Sunday-Monday)	23.75 GBP
Coffee	3.35 GBP
Sub-total	81.70 GBP
VAT @17.5%	14.30 GBP
Course notes	4.00 GBP
TOTAL	100.00 GBP

The fees of 100 GBP must be paid during registration in pounds sterling cash ONLY.

- Accommodation and meals are in St. Edmund Hall.
- The registration and the lectures are in the Nuclear Physics lecture room.
- IMPORTANT: Financial assistance towards your expenses depends where you are from. NOTE this is limited, so please apply as soon as possible if you need it.

UK participants only:

The EPSRC's Collaborative Computational Project on electronic structure (CCP9) will cover the workshop fee, so all you need to do at this stage is to state on the registration form that you need the workshop fees to be covered. There is also money for travel expenses, but you will have to apply for reimbursement directly to Dr Walter Temmerman at the Daresbury Laboratory on forms which will be provided at the workshop. To help us assess the cost of covering travel expenses, please indicate the cost of your travel on the registration form below.

USA participants only:

There is limited money for participants from the USA. The NRL in Washington has provided the workshop with funds to cover some fees and travel expenses. The workshop fees will be automatically taken care of at registration. To obtain reimbursement of travel expenses you must show us your tickets at registration. To help us allocate the travel money, please indicate the cost of your plane tickets in the registration form below. We will notify you of how much you can reclaim at the workshop by February 19th, 1996.

Non-UK and non-USA participants only:

We regret that we are unable to provide financial assistance.

Registration Form

NAME:
ADDRESS: ....

E-mail: ....

Telephone: .... FAX: ....

Do you need FINANCIAL ASSISTANCE towards:

(i) workshop fees (YES/NO)......................................

(ii) travel (YES/NO) ....

Cost of travel (if YES): ....

BOP96 WORKSHOP BACKGROUND READING TO TIGHT-BINDING THEORY AND METHOD OF MOMENTS

- DAVID PETTIFOR "BONDING AND STRUCTURE OF MOLECULES AND SOLIDS" (0-19-851786-6, 272 PP., 18.95 GBP, SOFT COVER).
- ADRIAN SUTTON "ELECTRONIC STRUCTURE OF MATERIALS" (0-19-851754-8, 276 PP., 17.85 GBP, SOFT COVER).

TO ORDER:

UK: credit card phone 01536-454-534
US: credit card phone 1-808-451-7556

Announcement

RESEARCH WORKSHOP ON CONDENSED MATTER PHYSICS

17 June - 23 August 1996

Working Group on Computational Electronic Structure: LOCAL DENSITY FUNCTIONAL AND BEYOND

17 - 28 June 1996

Within the framework of the 1996 Research Workshop on Condensed Matter Physics, a Working Group on COMPUTATIONAL ELECTRONIC STRUCTURE, centered on the topic "LOCAL DENSITY FUNCTIONAL AND BEYOND", will be held from 17 to 28 June 1996, at ICTP. The group will be directed by C.O. Rodriguez (IFLISYB, La Plata, Argentina), A. Mookerjee (S.N.Bose Centre, Calcutta, India), and J. Kohanoff (ICTP, Trieste, Italy).

The purpose of this Working Group is twofold: 1) to introduce the participants to modern (state-of-the-art) computational techniques for electronic structure calculations within the LD and LSD approximations to DFT, using the full potential LMTO methodology, and 2) to discuss and explore - with the guidance of experts in the relevant fields - several different proposals to improve the description of many-body effects beyond the LDA and LSDA.

The first week (17 to 21 June) will include a set of lectures on the basic theory, methodologies, applications and future trends, combined with hands-on tutorials on the actual implementation of the computer codes. The second week will be devoted mainly to tutorial sessions. However, some time will be reserved for the participants to present their own research accomplishments and interests. A stay of an additional two weeks could be envisaged for those participants developing a specific project within the topics covered in the Working Group.

A preliminary list of speakers includes:

- **M. Methfessel** (*Frankfurt an der Oder, Germany*): The FP-LMTO method and codes based on it for solids and molecular dynamics of clusters and molecules.
- **M. van Schilfgaarde** (*Menlo Park, California, USA*): Spin polarized calculations and magnetism.

- **A.Paxton** (*Belfast, Ireland*): Application of the FP-LMTO method to problems in materials science.
- **A. I. Liechtenstein** (*Stuttgart, Germany*): Beyond the LDA: LDA + U.
- **W. Temmerman** (*Daresbury, UK*): Beyond the LDA: LDA + SIC.
- **P. Weinberger** (*Vienna, Austria*): Screened (relativistic) KKR.

Applications from graduate students about to finish their PhD, fresh post-docs, and young active faculty members are encouraged. A background in solid state theory, electronic structure and density functional theory is required. Knowledge of FORTRAN programming language and UNIX environment is a necessary condition. This has to be clearly stated in the application.

Participation is open to all scientists from all member countries of the United Nations, IAEA or UNESCO. Registration is cost free. Please note: except for those participants selected for the Condensed Matter Research Workshop, there will be no special funds available for this Working Group. For funding under the European Commission, kindly refer to the Research Workshop Bulletin. Participation will be limited.

If you are interested in attending, please send by post/fax the Application Form for the Research Workshop on Condensed Matter Physics, including your full C.V. with a list of publications, one or more support letters from established scientists, and a short description of a scientific project which you plan to pursue after participation in this Working Group, directly to:

RESEARCH WORKSHOP ON CONDENSED MATTER PHYSICS
Working Group on Local Density Functional and Beyond
International Centre for Theoretical Physics
P.O. Box 586, I-34100 Trieste, Italy
Telephone: +39-(0)40-2240111
Telefax: +39-(0)40-224163
Telex: 460392 ICTP I

(This Announcement is also obtainable via e-mail: SMR928@ictp.trieste.it by typing on the subject line "get LOCAL DENSITY" or via Gopher Server: gopher.ictp.trieste.it Please note: Latex/Tex files are not accepted.)

The European Conference
PHYSICS OF MAGNETISM 96
June 24-28, Poznan, Poland

General information

The Conference **PHYSICS OF MAGNETISM 96** will be the eighth of the series organized, every three years since 1975, jointly by the Institute of Molecular Physics of the Polish Academy of Sciences and the Institute of Physics of the Adam Mickiewicz University in Poznan. The Conference is meant as an international forum for the presentation and discussion of novel scientific ideas, in a field of broadly understood magnetic phenomena, experimental results and new magnetic materials, with special emphasis on the following subjects:

- Electronic Structure
- Correlated Electrons
- Films, Multilayers and Nanostructures
- High-Tc Superconductivity

The main objective of the Conference is to bring together scientists and technologists from the Western, Central and Eastern European countries involved in research and application of new magnetic materials and high temperature superconductors. The conference is believed to contribute towards the scientific and cultural unification of Europe.

List of invited speakers

1. **B. Barbara**,
Laboratoire de Magnetisme Louis Neel, CNRS, Grenoble, France
"Quantum tunneling in magnets" (tentative).
2. **P. Bruno**,
Inst. d'Electronique Fondamentale, Universite Paris-Sud, Orsay, France
"Quantum size effect and related phenomena in ultrathin layered magnetic systems".
3. **P. Coleman**,
Physics Department, Rutgers University, Piscataway, N.J., USA

title to be announced.

4. **T. Dietl**,
Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
"Influence of magnetic impurities upon universal conductance fluctuations".
5. **V. Emery**, (to be confirmed)
Department of Physics, Brookhaven National Laboratory, Upton, USA
title to be announced.
6. **G.A. Gehring**
Department of Physics, University of Sheffield, U.K.
title to be announced.
7. **P.A. Gruenberg**,
Forschungszentrum Juelich-IFF, Juelich, Germany
"Layered magnetic structures in research and application".
8. **B.L. Györffy**,
H.H. Wills Physics Laboratory, Bristol University, Bristol, UK
"de Haas-van Alphen Oscillations in Superconducting State".
9. **J. Jensen**,
Physics Laboratory, H.C. Oersted Institute, Univ. of Copenhagen, Denmark
title to be announced.
10. **A. Jezierski**,
Inst. of Molecular Physics, Polish Academy of Sciences, Poznan, Poland
"Electronic structure and magnetic properties of intermetallic compounds".
11. **D. Johnston**,
Department of Physics and Astronomy, Iowa State University, Ames, USA
title to be announced.
12. **S. Kaprzyk**,
Inst. of Physics and Nuclear Techniques, Academy of Mining and Metallurgy, Krakow, Poland
"Spin density in real and momentum space in multiatom alloys by KKR-CPA method".
13. **J. Kirchner**,
Max-Planck Institut fuer Mikrostrukturphysik, Halle, Germany
title to be announced.
14. **P. Lindgard**,
Physics Department, Riso National Laboratory, Roskilde, Denmark
title to be announced.
15. **K. Roell**,
Gesamthochschule Kassel-Universitaet, FB Physik, Kassel, Germany
"Exchange coupled double layers for magneto-optical applications".
16. **T. Schneider**,
IBM Res. Division, Zurich Res. Lab., Rueschlikon/Zurich, Switzerland

"Evidence and Implication of XY-Critical Point Behaviour in Cuprate Superconductors".

17. **T. Shinjo**,
Institute for Chemical Research, Kyoto University, Japan
"Magnetism and magnetoresistance of multilayers prepared on microstructured substrates".

18. **H.L. Skriver**,
Lab. of Appl. Physics, Tech. Univ. of Denmark, Lingby, Denmark
"Magnetic interfaces and multilayers".

19. **F. Steglich**,
Institut fuer Festkoerperphysik, TH Darmstadt, Darmstadt, Germany
"Superconductivity, Magnetism and Non-Fermi-Liquid Effects in Strongly Correlated f-Electron Systems".

20. **T. Story**,
Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
"Correlation between electronic and magnetic properties in semimagnetic semiconductors".

21. **W. Suski**,
Inst. for Low Temperature and Structure Res., Polish Academy of Sciences, Wroclaw, Poland
"Magnetism of the Uranium Intermetallics".

22. **C. Varma**,
AT&T Bell Laboratories, Murray Hill, USA
title to be announced.

Contributed papers

Papers can be submitted either for poster or oral presentation. All abstracts will be refereed and the Organizing Committee will make a final decision on the assignment of papers to sessions and the presentation mode. The authors are asked to send 3 copies of a one-page abstract to the Conference Office prior to March 15, 1996 (full text before May 31, 1996; detailed information in the second circular).

The conference proceedings containing plenary talks and selected papers will be published as a special issue of Acta Physica Polonica A.

The length of the contributed papers will be limited to 4 printed pages.

The abstract should contain concise (up to 200 words) information about the content of the paper. It should be informative and not only indicate the general scope of the paper but also state the main results obtained and conclusions drawn. The abstract should be complete in itself.

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email: *rom@vm.amu.edu.pl*
(*R. Micnas – chairman*)

Announcement

PhD position at Martin-Luther-University Halle-Wittenberg

” Theory of magnetic nanostructures on metal surfaces ”

Applications are invited for one PhD position at the theory group of the Department of Physics, Martin-Luther-University Halle-Wittenberg (Germany), to be occupied as soon as possible.

The work will be devoted to ab initio electronic structure calculations of metallic nanostructures on metal surfaces. Special attention will be given to the interaction of small metallic clusters with imperfections of the surface.

The applicant should have good knowledge of theoretical solid state physics and experience with numerical calculations.

The salary will be approximately DM 1900 (1300 after tax and insurance). The appointment will be for two years first, with an option of prolongation if the work proceeds successfully.

For more information contact :

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Announcement

PhD in Theoretical Physics

Department of Physics, University of Exeter, Exeter,
EX44QL, UK

An EPSRC Ph. D position is immediately available for studies into theoretical investigations of the optical properties of rare earth impurities in silicon using *ab initio* local density functional theory. The student will join Dr. R. Jones' group and be expected to become familiar with large scale parallel computational techniques.

Interested parties should write to Dr. Jones of the above address or e-mail jones@excc.ex.ac.uk.

O(N) Multiple Scattering Method for Relativistic and Spin Polarised Systems

S.V. Beiden[a], G.Y. Guo[b], W.M. Temmerman[b], Z. Szotek[b],
G.A. Gehring[a], Yang Wang[c], G.M. Stocks[c], D.M.C. Nicholson[c],
W.A. Shelton[c], and H. Ebert[d]
[a] *Department of Physics, University of Sheffield, Sheffield, U.K.*
[b] *Daresbury Laboratory, Warrington, WA4 4AD, U.K.*
[c] *Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.*
[d] *Institute for Physical Chemistry, University of München, Theresienstr. 37, D-80333 München, Germany*

Abstract

We have implemented the fully relativistic and spin-polarised extention of the O(N) real space locally self-consistent multiple scattering formalism [1]. Here we present preliminary results for the spin and orbital magnetic moments and magneto-crystalline anisotropy in iron metal. The spin and orbital moments are in good agreement of conventional electronic structure methods. The preliminary results for the magneto-crystalline anisotropy have been obtained in the frozen potential approximation.

(submitted to Proceedings of MRS Fall Meeting, Boston, 1996)
Manuscripts available from: w.m.temmerman@dl.ac.uk

References

[1] D.M.C. Nicholson, G.M. Stocks, Y. Wang, W.A. Shelton, Z. Szotek, and W.M. Temmerman, Phys. Rev. B **50**, 14686 (1994).

Electronic Structure Studies of B2-Type Transition Metal Alumnides: Experiments and Theory

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Abstract

The electronic structure and bonding character of intermetallic alloys are investigated by a combination of electron energy loss spectroscopy (EELS) experiments and *ab initio* electronic structure calculations. A detailed comparison is made between experimental spectra and calculations. The changes in electronic structure within a transition metal alumnide series and also due to variations in composition and upon alloying are studied using EELS spectra. The Korringa-Kohn-Rostoker coherent-potential-approximation method and large supercell models are used to investigate changes in composition and the effect of dopants on the electronic structure.

(submitted to Proceedings of MRS Fall Meeting, Boston, 1996)
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THE MAGNETIC STRUCTURE OF $Cu_{0.2}Ni_{0.8}$ ALLOYS

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Abstract

The locally self-consistent multiple scattering method is applied to *ab initio* spin-polarized local density approximation calculations for ferromagnetic CuNi alloys. The samples used to model the alloys are constructed with experimentally measured short range order parameters. These large cell calculations are performed using the Intel Paragon XP/S massively parallel processing supercomputer. The neutron magnetic diffuse scattering cross sections are calculated and compared with experiment. The dependence of magnetic moment formation on the local environment is discussed.

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Origin of metallic surface core-level shifts

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Abstract

Using density-functional-theory we have calculated the surface core-level shifts (SCLSs) and the $\mathbf{k}_{||}$, symmetry-, and layer-resolved density of states (DOS) of the $4d$ fcc(001) transition-metal surfaces as well as of Sr and Ag. The DOS for the surface and substrate layers at $\mathbf{k}_{||} = \mathbf{0}$ and for the xy and $x^2 - y^2$ subbands can be accurately represented by a simple band model, that of a semi-infinite chain with nearest neighbor coupling and potential shifts V_1 and V_2 on the terminal and penultimate sites. It is shown that there is a nearly linear relation between the SCLSs in the initial-state approximation and the fitted surface potential shifts V_1 for both symmetries. The final state corrections do not significantly weaken the correlation. It has been argued that the position of the whole d-band relative to the Fermi level is the important surface parameter determining the surface chemical reactivity and that SCLSs can be used as a probe of the surface d-band shift (SDBS). Our results confirm that if the initial-state contributions to the shifts dominate, SCLSs provide a suitable quantitative measure of the surface d-band shift. They show that SCLSs originate from changes in the tails of the electron states at the surface.

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Latex(revtex/poscript) version can be obtained from: vero@fysik.dtu.dk

A Transferable Atomistic Model to describe the Energetics of Zirconia

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Abstract

We have investigated the energies of a number of phases of ZrO_2 using models of an increasing degree of sophistication: the simple ionic model, the shell model, the compressible ion model, and finally a model including quadrupole polarisability of the oxygen ions. The three structures which are observed with increasing temperatures are monoclinic, tetragonal, and cubic(fluorite). Besides these we have studied some hypothetical structures which certain potentials erroneously predict or which occur in other oxides, eg. the $\mathrm{PbO_2}$ structure and rutile. We have also performed *ab initio* density functional calculations with the full-potential Linear Combination of Muffin-Tin Orbitals method to investigate the cubic-tetragonal distortion. A detailed comparison is made between the results using classical potentials, the experimental data and our own and other *ab initio* results. The factors which stabilise the various structure are analysed. We find the only genuinely transferable model is the one including compressible ions and polarisability to the quadrupole level.

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Contribution of surface resonances to STM images: (110) surfaces of III-V compound semiconductors

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Abstract

Voltage-dependent scanning tunneling microscopy images are compared to *ab initio* electronic structure calculations to give evidence that surface resonances are vital for the explanation of STM images of InP, GaP, and GaAs(110). It is shown that the occupied dangling bond state dominates the images at negative voltages, but its counterpart, the empty dangling bond state, is only of relevance for small positive voltages. The empty state images are rather governed by empty resonances. We show that the conventional dangling bond picture is insufficient to explain the STM images.

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Magnetic Exchange Coupling of 3d Metal Monolayers on Fe(001)

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Abstract

We report systematic *ab initio* calculations for the magnetic moments, the magnetic coupling and the interlayer relaxation of the whole $3d$ transition–metal series (V, Cr, Mn, Fe, Co, Ni) as monolayers on the Fe(001) substrate. An energy analysis reveals that V and Cr prefer the layered antiferromagnetic coupling, Mn favors the c(2×2) ferrimagnetic superstructure and Fe, Co and Ni monolayers favor the ferromagnetic coupling to Fe(001). Cr and Mn on Fe exhibit a delicate interdependence of magnetism, film thickness and structure.

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Structural and electronic properties of liquid and amorphous carbon calculated via the fuzzy tight-binding Monte-Carlo method

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Abstract

The "fuzzy" TB-MC method is based on the idea that the energy of a new configuration need not to be calculated exactly, because a statistical error in the energy may be included in the thermal distribution via a new formulation of the Glauber dynamics of the Monte Carlo method. Depending on the method adopted for the calculation of the total energy, the computational effort scales between N^3 and N, where N stands for the number of electrons in the system. This allows to apply the technique to large systems. Applications of the new technique to the simulation of liquid and amorphous carbon at different densities are presented.

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Preprints available from: jhafner@tph.tuwien.at.ac

Atomic and electronic structure of diamond (111) surfaces:

I. Reconstruction and hydrogen-induced de-reconstruction of the one-dangling-bond surface

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Abstract

We present *ab-initio* local-density functional calculations of the atomic and electronic structure of the clean and hydrogen-covered one-dangling-bond diamond (111) surfaces. The calculations are based on a finite-temperature local-density approximation, optimized ultrasoft pseudopotentials, and an exact calculation of the electronic ground-state and Hellmann-Feynman forces before any step in the geometrical optimization of the surface. We find that the clean C(111) surface reconstructs in a $(2{\times}1)$ geometry with symmetric, unbuckled π-bonded Pandey chains. Although the surface chains are unbuckled and undimerized, we find a substantial buckling in the deeper layers. Our calculations show that there is essentially no energy-barrier against reconstruction. In equilibrium, a monolayer-coverage of hydrogen leads to a complete de-reconstruction with a slightly relaxed C(111)-$(1{\times}1)$:H surface. However, there is an appreciable energy-barrier against de-reconstruction. A reconstructed C(111)-(2×1):H surface can exist as a metastable configuration. For the clean reconstructed surface we predict both occupied and empty surface states in the bulk-gap, in good agreement with experiments. For both the stable unreconstructed and the metastable reconstructed hydrogenated surfaces we find that the hydrogen-saturation of the dangling-bond state shifts the surface-state to larger binding energies. Interaction with bulk-states leads to de-localization. We find that the hydrogenation induces a negative-electron-affinity effect on the C(111) surface.

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Preprints available from: jhafner@tph.tuwien.at.ac

(2×1) reconstruction and hydrogen-induced de-reconstruction of the diamond (100) and (111) surfaces

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Abstract

We present a comparative study of the (2×1) reconstruction of the (100) and (111) diamond surfaces, and of their hydrogen-induced de-reconstruction, using ab-initio local-density-functional calculations. We show that whereas for the (111) surface the absorption of a monolayer of hydrogen stabilizes the (1×1) bulk-terminated surface, for the (100) surface the (2×1) surface structure remains stable (albeit with a strongly enhanced bond-length of the surface dimers). Results for the electronic surface-states are presented.

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Surf. Sci. (in print))
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Ab-initio Force-Constant Approach to Phonon Dispersion Relations of Diamond and Graphite

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Abstract

The phonon dispersion relations of diamond and graphite are calculated using an *ab-initio* force constant method. The force constants are calculated via a selfconsistent supercell approach in the local-density approximation in terms of the Hellmann-Feynman forces induced by the displacement of a single atom in the supercell. For diamond our *ab-initio* results are in very good agreement with the neutron inelastic scattering and Raman data. For graphite we find good agreement with the neutron data for the low-energy-modes as well as with the reflections electron energy loss spectroscopy (REELS) and optical data at higher energies. Significant differences to the predictions of semiempirical models appear.

Europhys.Lett. 32(1995)729.
Reprints available from jhafner@tph.tuwien.ac.at

Ab-initio simulation of the metal/nonmetal transition in expanded fluid mercury

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Abstract

We present an investigation of the variation of the structural and electronic properties of liquid mercury for states along the liquid-vapour coexistence line, spanning the range from the triple-point to the critical point. Our study is based on ab-initio density-functional molecular dynamics on the Born-Oppenheimer surface. Of central interest is the metal/nonmetal transition occurying at densities approximately twice the critical densities. Our results show that the metal/nonmetal transition is best described as a simple band-crossing transition and that electron localization and many-body effects are not essential.

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Disorder and non-collinear magnetism in permanent-magnet materials

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Abstract

We report calculations of the non-collinear magnetic structures and of the magnetic anisotropies of $\mathrm{YFe}_{12-x}\mathrm{Mo}_x$ permanent magnets with the ThMn_{12} structure, using a novel variant of a spin-polarized tight-binding–linear-muffin-tin-orbital technique allowing for local spin-quantization axes on each site and considering spin-orbit coupling. The ternary $\mathrm{YFe}_{12-x}\mathrm{Mo}_x$ compounds crystallize in the tetragonal ThMn_{12} structure which can be stabilized only by the partial substitution of Fe by an early transition metal like Mo. We show that the substitutional disorder leads to canted spin-structures at low Mo-content (x $\sim$ 1) and to spin-glass-like behavior at higher Mo-content (x $\sim$ 3). We also find that the character of the anisotropy changes from uniaxial to planar with higher Mo content.

(MMM-Conference 1996, J.Appl.Phys. (in print))
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ELECTRONIC STRUCTURE OF ICOSAHEDRAL AND DECAGONAL AL-PD-MN ALLOYS

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Abstract

We present calculations of the electronic structure of icosahedral and decagonal Al-Pd-Mn alloys, based on a hierarchy of rational approximants to realistic quasicrystalline structures and the linear-muffin-tin-orbital (LMTO) and tight-binding LMTO methods. For the icosahedral phase we show that a structure-induced density-of-states minimum at the Fermi-level exists for the stable 2/1 and all other higher-order approximants, but not for the lowest-order 1/1 phase. We also present preliminary results for the decagonal phase and show that the electronic structure is similar to that of the icosahedral alloy.

(Proc. 5th Intern. Conference on Quasicrystals (Avignon 1995), in print)
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Magnetic anisotropies of thin fcc Fe-layers on Cu(100)

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Abstract

We present ab-initio calculations of the spin-structures and the magnetic anisotropies of face-centred-cubic iron films on Cu(100) substrates with the thickness varying between one and six monolayers. The calculations are based on a self-consistent tight-binding linear-muffin-tin orbital method with variable local spin quantization axes. Our calculations show that for films with more than three monolayers, the magnetic polarizations of the films acquires an antiferromagnetic component, for films with more than four monolayers metastable magnetic configurations appear. For the fcc Fe monolayers we predict a perpendicular anisotropy on Cu(100) and an in-plane anisotropy on Cu(111). For the thicker layers on Cu(100) we find a decreasing perpendicular anisotropy for up to six monolayers, we expect a transition to in-plane anisotropy for 8 to 10 monolayers.

(Proc. 6th European Conf. on Magnetic Materials (EMMA6), J.Magn.Magn.Mat. (in print))
Preprints available from: jhafner@tph.tuwien.at.ac

Are decagonal quasicrystals Hume-Rothery alloys ?

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Abstract

The possible importance of a Hume-Rothery mechanism for understanding the stability of decagonal quasicrystals is discussed on the basis of selfconsistent calculations of the electronic structure of higher-order approximants to decagonal and icosahedral Al-Pd-Mn alloys, as well as some related crystalline phases.

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Local spin-density theory of spin-glasses

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Abstract

We present ab-initio calculations of the spin-structures for the "spin-glass" alloys $Cu_{95}Mn_5$ and $Cu_{90}Mn_{10}$, based on the local spin-density approximation (LSDA) and a supercell-approach. The calculations are performed using the linear-muffin-tin-orbital (LMTO) technique with collinear spins (corresponding to a Ising-type model) as well as a tight-binding-LMTO technique allowing for arbitrary orientations of the local spin-quantization axes (corresponding to a Heisenberg-type modell). Our calculations predict a spin-glass-like magnetic ground-state. The spin-disorder arises from a competition of predominantly antiferromagnetic nearest-neighbour interactions with a ferromagnetic coupling to the more distant neighbours.

(Proc. 6th European Conference on Magnetic Materials (EMMA6), J. Magn. Magn. Mat. (in print))
Preprints available from: jhafner@tph.tuwien.at.ac

The structural and electronic properties of rhodium surfaces: An ab-initio approach

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Abstract

The structural and electronic properties of the low-index surfaces of Rhodium have been investigated via fully self-consistent *ab-initio* local-density-functional (LDF) calculations. Our technique is based on ultrasoft pseudopotentials, a preconditioned conjugate-gradient technique for the calculation of the electronic ground-state and of the Hellmann-Feynman forces and stresses, and on a conjugate-gradient technique for the optimization of the atomic structure. The calculations were performed for five- to ten-layer slabs in symmetric and asymmetric geometries, allowing for the relaxation of up to seven surface layers. For the (111), (100), and (110) surfaces an inward relaxation of the top layer by -1.7 ± 0.2, -3.8 ± 0.2, and $-9.8 \pm 0.6\%$ is predicted, the surface-energies increase parallel to the inward-relaxation. The analysis of the electronic structure shows that the inward-relaxation is caused by the de-population at the surface of anti-bonding states at the top of the d-band. We also present a detailed analysis of electronic surface states.

(Surf.Sci. 346 (1995) 300)
Reprints available from: jhafner@tph.tuwien.at.ac

Surface reconstruction and electronic properties of clean and hydrogenated diamond (111) surfaces

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Abstract

We present *ab-initio* local-density-functional calculations of the structural and electronic properties of clean and hydrogenated diamond (111) surfaces with one and three dangling bonds (1db, 3db), respectively. For the clean 1db-surface we predict a (2×1) reconstruction with symmetric, very slightly buckled dimers at the surface, and a stronger buckling in the deeper layers. Hydrogenation leads to a complete de-reconstruction of the (111)-1db surface. For the 3db-surfaces we have performed a comparative study of the $(2{\times}1)$ and $(\sqrt{3} \times \sqrt{3})$ reconstructions and find the $(2{\times}1)$ structure to have a slightly lower energy for both the clean and the hydrogenated surfaces.

(Proc. 9th Intern. Conference on Surface Science (ICSS9, Yokohama 1995), Surf.Sci. (in print))

Preprints available from: jhafner@tph.tuwien.at.ac

First principles simulation of grain boundary sliding

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Abstract

We present the results of a total–energy pseudopotential simulation of the sliding process at a Σ=5 (001) twist grain boundary in germanium. Sliding involves a stick–slip mechanism with local rebonding among a few atoms, accompanied by the clearance of gap states. At large strain, spreading of disorder from the boundary interface produces a loss of strength in the system and would induce fracture. Finally we investigate the effects of temperature and strain rate on the sliding behaviour.

(to appear in Phys. Rev. Lett.)
The REVTEX version can be obtained from: cm10020@phy.cam.ac.uk

Stability of Na_nPb ($n \leq 7$) clusters: a first principles molecular dynamics study

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Abstract

The structural and electronic properties of bimetallic clusters Na_nPb ($n \leq 7$) are calculated by means of a first principles molecular dynamics simulated annealing using the local-density approximation and the pseudopotential plane-wave method. We obtain that the observed exceptional abundance of Na_6Pb in molecular beams is due to the combination of electronic and geometrical factors, which are absent in the case of $n \neq 6$ clusters. In particular we find that adding another Na atom to Na_6Pb is energetically less favorable than adding it to a pure Na cluster in contrast to what we obtain for smaller Na_nPb clusters.

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First-principles calculation of the anomalous perpendicular anisotropy of a Co monolayer on Au(111)

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Abstract

We perform fully-relativistic spin-polarized local spin density calculations for Au covered Co monolayer on Au(111). In very good agreement with experiments we obtain the enhancement of perpendicular magnetic anisotropy as a function of the Au coverage. The relation between the orbital magnetic moment anisotropy and the band energy anisotropy is also studied and compared to the predictions of tight-binding model calculations.

(submitted to Phys. Rev. Lett.)
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"Band structure" and electrical conductivity of disordered semi-infinite systems

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Abstract

Employing the Kubo-Greenwood formula the electrical conductivity of disordered semi-infinite systems is formulated in terms of the (Screened) Korringa-Kohn-Rostoker method and the Coherent Potential Approximation. It is shown that by neglecting vertex corrections in the same manner as in the bulk case, the elements of the electrical conductivity tensor can be described in terms of "layer-diagonal"- and "layer-off-diagonal" contributions. In order to discuss effects of the underlying electronic structure on the electrical conductivity, but also to point out particular contributions to it, Bloch spectral functions are formulated. A spin-polarized (relativistic) application of the present theory to non-collinear disordered magnetic multilayers allows to discuss giant magnetoresistance (GMR) on an ab-inito level in quite a general context.

(submitted to J.Phys.Cond.Matt.)
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A new type of oscillatory exchange coupling induced by ordering in the magnetic layers

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Abstract

We found that formation of an ordered phase in alloyed magnetic layers induces new periods of exchange coupling oscillations in metallic multilayer systems. We studied on an ab-initio level the case of c(2×2) ordering of random $Co_{50}Fe_{50}(001)$ magnetic slabs embedded in fcc-Cu. The origin of the new periods can be correlated to critical points of the spacer Fermi surface folded down to the Brillouin zone corresponding to the c(2×2)-superlattice.

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

GROUND STATE PROPERTIES AND STRUCTURAL PHASE TRANSFORMATION OF BERYLLIUMSULPHIDE

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Abstract

The electronic structure, the charge density and the total energy of BeS in the rocksalt (B1), cesiumchloride (B2), zincblende (B3), wurtzite (B4), nickelarsenide (B81) and ironsilicide (B28) structures are studied using first-principles self-consistent local- density calculations in a large plane wave basis employing soft non-local pseudopotentials. The zincblende structure is the calculated ground state with a=4.773 , B0=101.9 GPa and B0'=3.70. The experimental value is a=4.85 . The wurtzite structure is energetically very close to the zincblende structure. The difference at the minimal energy in these two structures is only 6.2 meV. At a pressure of 58 GPa we observe a transition to the six-fold coordinated nickelarsenide structure. From that structure on no other transition is found to any of the calculated structures.

(submitted to Sol.Stat.Comm.)
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Ab initio Electronic Structure, Magnetism and Magnetocrystalline Anisotropy of UGa_2

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Abstract

Ab initio electronic structure calculations for the intermetallic compound UGa_2 were performed using an optimized LCAO (linear combination of atomic orbitals) method based on the local spin density approximation. Three separate calculations were done treating the uranium 5f states as band states and as localized states with occupation two and three, respectively. In the itinerant approach, spin and orbital moments, magnetocrystalline anisotropy, and Sommerfeld constant were calculated and found to deviate significantly from the related experimental data. In the localized approach, crystal field parameters were obtained for the 5f states which have been treated by self-interaction corrected local density theory. This approach with $5f^2$ occupation is shown to provide reasonable results for the anisotropy of the susceptibility, for the field dependence of the magnetic moments, and for the Sommerfeld constant.

(accepted to Phys. Rev. B)

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Defect Interactions in Al

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Abstract

We present systematic *ab initio* local-density-functional (LDF) calculations for defect interactions in Al. In particular, we calculate interaction energies of both impurity-vacancy and impurity-impurity pairs on first and second neighbor sites; as impurities, we choose Sc-As (3*d* and 4*sp* series) and Y-Sb (4*d* and 5*sp* series). The present method is based on the Kohn-Korringa-Rostoker Green's-function method and treats the impurity problems without approximations such as the pseudopotential method and the supercell approach. The calculations reproduce well the experimental values for the vacancy-solute interaction and elucidate the micromechanisms of the vacancy-impurity and impurity-impurity binding energies.

(submitted to Phys. Rev. B)
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Structural and Magnetic Phase Stability of VS and VSe

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Abstract

Using the full potential linear augmented plane wave (LAPW) band structure method a detailed investigation of the structural and magnetic phase stability of VS and VSe, respectively, has been performed. In full accordance with experiment the MnP-structure was found to be the equilibrium phase for VS at low temperature. The changes in the electronic structure that accompany the phase transition from the orthorhombic MnP– to the hexagonal NiAs-structure is monitored using the dispersion relations, the density of states curves as well as the electronic charge density distribution. For VSe in the NiAs-structure the magnetic phase diagram as a function of the hexagonal lattice parameter a and c has been determined. In agreement with experiment, the antiferromagnetic phase was found to be energetically the most favourable one among the para–, ferro– and antiferromagnetic phases.

(submitted to Journal of Alloys and Compounds)
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Spin-orbit interaction and spontaneous galvanomagnetic effects in ferromagnetic alloys

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Abstract

The dependency of the isotropic residual resistivity and of the galvano-magnetic effects on the various relativistic effects has been studied for permalloy $Fe_{0.2}Ni_{0.8}$. For the isotropic resistivity the two-current model was found to break down because of the influence of the spin-orbit coupling. While the so-called scalar relativistic effects were found to have a small influence on the isotropic resistivity they are unimportant for the spontaneous magnetoresistance anisotropy and anomalous Hall resistivity. These spin-orbit induced effects turned out to vary roughly quadratically with the spin-orbit coupling strength.

(submitted to Solid State Communications)
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L-Edge X-Ray Absorption in fcc and bcc Cu Metal: Comparison of Experimental and First-Principle Theoretical Results

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Abstract

High resolution Cu $L_{2,3}$ x-ray absorption spectra of bulk fcc Cu metal are compared with those of thin Cu layers in Cu/Fe multilayers. Comparison of the measured fine structure with that obtained from a fully relativistic first principles calculation for fcc and bcc Cu reveals that Cu is bcc in Cu(3Å)/Fe(10Å) and fcc in Cu(10Å)/Fe(3Å) multilayers. This result indicates that the thicker layer simply acts as a template for the structure of the thinner layer. The excellent agreement between experimental and theoretical spectra also demonstrates the validity of the theoretical approach. The theoretical spectra are discussed in terms of their angular momentum composition and the energy dependence of the radial transition matrix elements.

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Invertible and non-invertible alloy Ising problems

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Abstract

Physical properties of alloys are compared as computed from "direct" and "inverse" procedures. The direct procedure involves Monte Carlo simulations of a set of local density approximation (LDA)-derived pair and multibody interactions $\{\nu_f\}$, generating short-range order (SRO), ground states, order-disorder transition temperatures, and structural energy differences. The inverse procedure involves "inverting" the SRO generated from $\{\nu_f\}$ via inverse-Monte-Carlo to obtain a set of *pair only* interactions $\{\tilde{\nu}_f\}$. The physical properties generated from $\{\tilde{\nu}_f\}$ are then compared with those from $\{\nu_f\}$. We find that (i) inversion of the SRO is possible but, (ii) the resulting interactions $\{\tilde{\nu}_f\}$ agree with the input interactions $\{\nu_f\}$ only when the problem is dominated by *pair* interactions. Otherwise, $\{\tilde{\nu}_f\}$ are *very* different from $\{\nu_f\}$. (iii) The same SRO pattern can be produced by drastically different $\{\nu_f\}$. Thus, the effective interactions deduced from inverting SRO are not unique. (iv) Inverting SRO always misses configuration-independent (but composition-dependent) energies such as the volume deformation energy $G(x)$; consequently, the ensuing $\{\tilde{\nu}_f\}$ cannot be used to describe formation enthalpies or two-phase regions of the phase diagram, which depend on $G(x)$.

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First-principles LSDF study of weak ferromagnetism in Fe_2O_3

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Abstract

We report results of calculations that explain in the itinerant electron picture weak ferromagnetism in hematite, α-Fe_2O_3. We use the local approximation to spin-density functional theory and the ASW method incorporating spin-orbit coupling (SOC) and noncollinear moment arrangements. By a detailed symmetry analysis we show how the relativistic effect of SOC and the particular crystal symmetry of α-Fe_2O_3 cooperate to lead to a noncollinear magnetic structure and thus to weak ferromagnetism.

(To appear in Europhysics Letters)
Revtex version can be obtained from: dg5m@mad1.fkp.physik.th-darmstadt.de (L. Sandratskii)

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Spin-Orbit Influenced Spectroscopies of Magnetic Solids

H. Ebert and G. Schütz (Eds.)
Proceedings of the International Workshop on
Spin-orbit influenced spectroscopies of magnetic solids,
held at Herrsching, Germany, April 20 - 23, 1995
Lecture Notes in Physics, Volume 466, March 1996
Springer-Verlag, Berlin

Preface

The increasing availability of synchrotron radiation with high intensity and well-defined polarization over a wide range of photon energies allowed the refinement and extension of all kind of electronic spectroscopies during the last 10 – 15 years. As has been proven by the emission of spin-polarized photoelectrons from paramagnetic solids excited by circularly polarized light, spin–orbit coupling is intimately interwoven with magnetism and can give rise to quite peculiar phenomena. For this reason it is not astonishing at all that the above–mentioned development has an especially great impact on the electronic spectroscopy of magnetic solids. In particular it gives access to very detailed experimental studies of the complex and fascinating interplay of spin–orbit coupling and magnetic ordering that accordingly require a corresponding thorough theoretical description.

This book collects a number of selected and representative lectures given at a workshop on *Spin–orbit influenced spectroscopies of magnetic solids* held from 20 to 23 April 1995 at the Bildungsstätte des Bayerischen Bauernverbandes at Herrsching, Germany. The purpose of this workshop was to bring together experimental and theoretical researchers in this rapidly developing field to present and discuss their latest results. Accordingly it was a meeting of most members of the network *Novel probes for magnetic materials and magnetic phenomena: linear and circular X-ray dichroism* coordinated by A. Fontaine (Grenoble) and set up within the *Human Capital and Mobility* (HCM) programme of the EU. Most of the other participants working on the theory of electronic spectroscopy were members of the HCM network *Ab initio (from electronic structure) calculation of complex processes in materials* coordinated by W. Temmerman (Daresbury).

The most important electronic spectroscopies used today for investigations of the properties of magnetic solids were dealt with during the workshop and in general on each topic there was at least one experimental and one theoretical contribution. The magneto-optical Kerr effect in the optical regime of light – known for more than a century – exemplifies that spin–orbit-influenced spectroscopies can be of technical importance. In spite of the strong and broad interest in this effect a thorough and quantitative theoretical description became possible only during the last few years. A rather direct and detailed method for investigating the hybridisation of valence band states of different spin character caused by spin–orbit coupling – the primary source for the magneto-optical Kerr effect – is supplied by the spin- and angle-resolved photoemission spectroscopy. Again theory has proven extremely successful in describing the corresponding spectra and in explaining the various dichroic phenomena. In particular the consequences of the reduced symmetry due to the simultaneous occurrence of spin–orbit coupling and magnetic ordering can be discussed in great detail. Spin- and angle-resolved core–level photoemission spectroscopy is a somewhat indirect tool for studying magnetic properties. Nevertheless it gives interesting additional and above all component-specific information. As in the situation for f-electron systems, a localized or atomic-like picture of the relevant electronic properties seems often to be more adequate than the model of itinerant magnetism used for the Kerr and valence–band photoemission spectroscopy of transition metals. As for the core–level photoemission spectroscopy, X-ray absorption spectroscopy supplies component–resolved information. Although this kind of spectroscopy maps the unoccupied states above the Fermi level it nevertheless can be used to get an estimate for the spin as well as the spin–orbit–induced orbital magnetic moments of the absorbing atom. This can be achieved with the help of approximate sum rules derived during the last few years. In addition, theory allows for a detailed discussion of the corresponding absorption spectra and their dependency on the polarization of the radiation, i.e., the magnetic dichroism and their relationship to the underlying microscopic electronic structure. A very interesting application of dichroic effects in X-ray absorption is the investigation of domain structures and magnetic coupling at interfaces – which can be done in a component resolved way. This also applies to the inverse experiment, i.e., to the X-ray emission that probes the occupied valence–band states. Although the corresponding measurements are quite hard to perform the first results seem to be quite promising and completely in accordance with the accompanying theoretical work. While conventional EXAFS supplies geometrical information on the neighborhood of the absorbing atoms its magnetic counterpart, making use of circularly polarized radiation, reflects the magnetic properties of the surroundings. Corresponding theoretical models became available recently by an extension of EXAFS theory as done before for the low-energy XANES region. X-ray anomalous scattering is also a relatively new tool for studying the magnetic properties of solids. Accompanying theoretical investigations allow for a detailed interpretation of such experiments and allows us to unveil its relationship with other spectroscopies.

The workshop was made possible by financial support from the network *Relativistic effects in heavy element chemistry and physics* of the European Science Foundation (ESF), coordinated by P. Pyykkö (Helsinki) and B. Hess (Bonn), as well as the HCM network *Ab initio (from electronic structure) calculation of complex processes in materials* coordinated by W. Temmerman (Daresbury). We would like to thank these organisations and their coordinators for their generous support. Furthermore we thank all contributors and participants for making the workshop a successful one and for the realization of these proceedings. Finally we acknowledge the efforts of M. Battocletti, H. Freyer, V. Popescu, J. Schwitalla, and A. Vernes in preparing the final LaTeX versions of the manuscripts.

Munich, Augsburg H. Ebert and G. Schütz

December 1995

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HIGHLIGHTS OF 1995

In this section we present scientific highlights of some of the Network's collaborations for the past calendar year.

Large Systems and Pseudopotentials: Pulling a piece of aluminium apart

by Volker Heine
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(Cambridge–Stuttgart Collaboration)

In recent decades, much research has focused on the properties of glamorous materials such as silicon and other semiconductros, magnetic layers, high temperature superconductors and many more. However the heart of materials science still lies in a sense in the mechanical strength of materials: why does the bridge not fall down, or rather how much money can be saved by making the girders thinner? The matter of mechanical strength is scientifically a difficult one, not only because of the complexity of the processes occurring in deformation and fracture, but because they span two length scales: the atomic scale of Angstroms and the mesoscopic scale of microns.

Both length scales are essential. The stress field around a crack tip and generation of dislocations belong to the mesoscopic scale, while fracture ultimately means overcoming the interactomic bonding forces on the atomic scale. It is in the latter where one might expect to see the difference between the brittle covalently bonded materials and ductile metals with atoms held by metallic bonding. Actually such a view was rather unfashionable until recently. It was thought that the only role of the interatomic forces was to determine the crystal structure, e.g. face centred cubic for many metals and, say, the diamond structure for silicon. After that, it was the propensity of the crystal structure to dislocation slip that was the dominant factor in ductile or brittle behaviour.

While that remains a large part of the answer, the actual interatomic forces at a crack tip have also been shown to matter in recent ab initio quantum mechanical calculations. In metallic bonding the atoms are relatively free to slide over one another as long as the total coordination number is approximately maintained. This can be seen in the calculations on aluminium by Deyirmenjian, Payne, Lynden-Bell and Heine in Cambridge with Finnis at the Max Planck Institute for Metallurgy in Stuttgart. The computer sample of aluminium had rows of missing atoms, the rows about 1.6 nm apart, each such row being a defect something like an incipient crack. The sample was pulled gradually in one direction until near failure at an extension of 28%, the full quantum mechanics for the electron bonding and the atomic positions being solved at every small increment of the extension process.

Several interesting points could be seen in the simulations, but there were two findings of wider significance. The first concerns the role of metallic bonding. Whereas the quantum calculation for aluminium clearly gave ductile behaviour even at zero degrees Kelvin, a parallel calculation using a pairwise Morse interatomic potential gave brittle failure with identical geometry. The special nature of metallic bonding is therefore important in ductile behaviour. The second achievement was a basic improvement in the empirical Sutton-Chen model of metallic bonding for aluminium. The number of atoms (per superlattice cell) needed to simulate real deformation processes in a computer sample is too large to be treated by the ab initio quantum mechanical methods, so that one is forced to use empirical classical models of the interatomic bonding. Since the work of Finnis and Sinclair in 1984, a series of models have been devised to represent metallic bonding. Collectively sometimes called glue models, they incorporate approximately the quantum effects and are enormously better than the models preceding them. Deyirmenjian tested one of these due to Sutton and Chen in a parallel calculation, again with the identical starting geometry as the quantum simulation. It also showed ductile fracture, but with a long strong precursor effect in the deformation around the line of vacancies which was absent in the proper quantum calculation. In sp bonded metals, a quantity of basic importance is the local volume per atom available to the bonding conduction electrons. Finnis has recently developed a good definition and computable algorithm of the local atomic volume in an arbitrary configuration, and when this was used to modify the attractive 'glue' term in the Sutton-Chen model, the precursor disappeared almost completely. We therefore have here a guide for developing better glue models in the future, and the quantum calculation represents a large database with which empirical models can be compared. However it must be admitted that the accumulating experience is that empirical models will never do a really good job, no matter how well they are tuned up. But we must use them for many many simulations too large to be treated by the full quantum mechanical calculations, and therein lies a love/hate relation between the two approaches.

Where is the Cooper Force in the High Temperature Superconductors

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(Bristol–Daresbury–Stuttgart Collaboration)

Eight years after the discovery of the High Temperature Superconductivity the physical mechanism behind this remarkable phenomenon remains a mistery. Many ingenous ideas have been tried [1] but so far they have failed to convince anyone except their inventors and their research students. Under these circumstances it may be worthwhile to approach the problem piecemeal, taking small steps at a time. Namely, one may attempt to isolate features of the problem which can be tackled without requiring a full solution. For instance, one might regard the establishement by Gough et al. [2] that the new superconductors, like the conventional ones, have to do with pairing of electrons, as the first move along this line. A similar but more dramatic step forward is the emerging consensus that the relative symmetry of the pair is d-type [3]. In this note we wish to highlight a new strategy for what might be an another useful manoeuvre. The aim is to determine at which site and in which state the members of a Cooper pair must be to experience the pairing force, without specifying its physical origin.

The approach is made possible by the particularly simple general form the attractive electron-electron interaction takes in the Density Functional Theory for superconductors [4]. Its pairing kernel $\lambda(\mathbf{r},\mathbf{r}';\mathbf{r_1},\mathbf{r}'_\mathbf{1})$ is given by functional derivatives of the exchange-correlation energy functional, of the charge density $n(\mathbf{r})$ and the pairing amplitude $\chi(\mathbf{r},\mathbf{r}')$, with respect to the pairing amplitude. The superconducting analogue of the usual Kohn-Sham equations has the general form of the Bogolubov-de Gennes equations which involve the pairing potential $\Delta(\mathbf{r},\mathbf{r}')$. The latter is determined through the pairing kernel $\lambda(\mathbf{r},\mathbf{r}';\mathbf{r_1},\mathbf{r}'_\mathbf{1})$ in terms of the pairing amplitude $\chi(\mathbf{r},\mathbf{r}')$ as follows

$$\Delta(\mathbf{r},\mathbf{r}') = \int \mathbf{d^3r_1} \int \mathbf{d^3r'_1}\lambda(\mathbf{r},\mathbf{r}';\mathbf{r_1},\mathbf{r'_1})\chi(\mathbf{r_1},\mathbf{r'_1}). \qquad (1)$$

Evidently, the great unknown in this theory is the pairing kernel, λ, which is, in general, a functional of both $n(\mathbf{r})$ and $\chi(\mathbf{r},\mathbf{r}')$. Our semi-phenomenological approach is to express λ in terms of site- and orbital-dependent coupling constants which are treated as adjustable parameters and determined by fitting to experimental data from such searching probes as photoemission, spin-lattice relaxation rates, and neutron scattering experiments.

What lends impetus to this strategy is the conjunction of two fortunate circumstances. On the one hand, a relatively small set of coupling constants describes a rather large class of mechanisms, and on the other, because these adjustable parameters are embedded in a fully first-principles calculation, a very large number of observables can be calculated without further adjustable parameters. Remarkably, when a set of coupling constants has been identified as being consistent with a variety of experiments, we have determined the orbital character and spatial location of the Cooper force without knowing its origin. Our hope is that such information will be suggestive concerning its nature.

A uniquely convenient starting point for our strategy is the eight-band model of Andersen et al. [5]. This model has the following features: **a)** it describes a Cu–O bilayer which is characteristic of many high T_c superconductors **b)** it has been obtained from first-principles (LMTO) calculations by a well controlled folding-down procedure **c)** it is of a required tight-binding form **d)** and finally, it has been shown to give a good quantitative account of the electronic structure, near the Fermi energy, in the normal state.

As a first step towards implementing the strategy outlined above, we have solved self-consistently the Bogolubov-de Gennes equations, corresponding to the eight-band model, for some 20 different choices of the coupling constants, and compared the resulting excitation spectra with those deduced from photoemission experiments [6]. In most cases we have studied we have assumed at most two different and non-zero coupling constants, with all the others set to zero. Concerning gap anisotropy, we have been able to assign a specific pairing interaction to each of the three different experimental scenarios for the superconducting gap anisotropy [7]. In particular, a gap of a zero value and a cusp along the (π, π) direction have been interpreted as arising from the nearest neighbour Cu $d_{x^2-y^2}$–Cu $d_{x^2-y^2}$ pairing interaction of 0.67 eV. A gap which is zero and a minimum along the (π, π) direction has been identified with the nearest neighbour Cu s–Cu $d_{x^2-y^2}$ pairing interaction of 2.3 eV, and finally, the most 'exotic' gap with a "hump" along the (π, π) direction has come out as a combined effect of the nearest neighbour Cu s–Cu $d_{x^2-y^2}$ pairing interaction of 2.7 eV and the nearest neighbour Cu p–Cu $d_{x^2-y^2}$ pairing interaction of 0.45 eV. Considering the magnitude of the pairing interaction of each studied case, the obvious favourite has to be the nearest neighbour Cu $d_{x^2-y^2}$–Cu $d_{x^2-y^2}$ pairing interaction, leading to a gap of d-type symmetry; which incidently is in line with the recently emerging consensus concerning the symmetry of the gap. Although we have been able to identify several different pairing interactions which also lead to a gap of d-type symmetry, their considerably larger magnitudes have inclined us to regard them, for the time being, as less physically likely. Thus, with some exaggeration to illustrate how our strategy can be useful, it can be said that we have deduced that the Cooper force operates between electrons on the nearest neighbour, in plane, Cu-sites and in the $d_{x^2-y^2}$ orbitals.

Interestingly, it is very difficult to reproduce the observed d-wave pairing with electrons on different Cu–O planes as required by the Anderson mechanism [1]. On the other hand, it is easy to imagine that the nearest neighbour Cu $d_{x^2-y^2}$–Cu $d_{x^2-y^2}$ pairing interaction is due to antiferromagnetic fluctuations. However, it is too early to draw firm conclusion from these preliminary results. Clearly, to lend further credence to this approach we must go on to calculate the other observables we have mentioned at the beginning of this note. Particularly promising are calculations of the spin lattice relaxation rates, $1/T_1$, at the Cu-, O-, and other-sites. Since no further adjustable parameters are required, these should decisively eliminate a number of contending interactions.

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Magnetic Impurities in Alkali Metals

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(Jülich–Athens Collaboration)

At a first sight the magnetic properties of transition metal impurities in alkali or alkali–earth metals do not seem to be particularly exciting. As it is well known, 3d impurities like Mn or Fe are magnetic in noble metal hosts, having a local magnetic moment at the impurity site and showing a Kondo behaviour at low temperatures. Why should it be interesting to introduce a 3d impurity in one of the alkali metal hosts with their much larger volumes, when the same impurity is already magnetic in Cu?

The interesting new aspect is the development of an orbital moment, as requested by Hund's second rule for free atoms. In the dense noble metals the orbital moment of the 3d impurities is quenched due to the strong hybridization of the d–wavefunctions with the s electrons of the host. Now, in the alkali metals with their very low electron density the Fe atom acquires in addition to the spin moment also an orbital moment. This is basically the same localisation transition which is well known from the rare earth and actinide systems. In fact, one might take any impurity from the transition metal series and insert it into any of the alkali metals, the volumes of which change quasicontinuously in the sequence Cu, Ag, Li, Na, K, Rb, Cs by a factor of 10. Thus in these systems one can study the transition to the atomic limit in great detail and for many different impurities.

This field has been pioneered experimentally by D. Riegel of the Hahn–Meitner Institut in Berlin. He introduced the transition metal impurities into the alkali metals by ion–implantation, since the natural solubility for these elements is vanishingly small. Using nuclear spin rotation techniques he obtained a rich variety of interesting physical properties, of which we will only mention two: i) While 3d impurities normally have both spin– and orbital moments, in certain cases, e.g. for Fe in Na or K, two configurations are found, a substitutional Fe atom with fully developed spin and orbital moments and in addition an interstitial Fe with spin moment only. Apparently the higher electron density at the interstitial site quenches the orbital moment. ii) Gross and Riegel [1] find that also 4d impurities like Mo, Tc and Ru show in the heavier alkali metals a nearly atomic behaviour with spin and orbital moments.

This work motivated us to perform ab–initio calculations for transition metal impurities in alkali metals [2]. Based on the local density approximation the calculations partly apply the KKR–Green's function method, partly they adopt the more simpler jellium model. The electronic structure of all 3d and 4d impurities in all monovalent metals has been considered. For the 3d impurities very strong local moments are obtained, being practically saturated. Even the impurities at the beginning and end of the transition metal series, i.e. Sc and Ni, become magnetic in the heavier alkali metals. 4d impurities show nearly the same strong magnetic tendencies as 3d ones. For instance, Mo has in K, Rb and Cs a local moment of about 5 μ_B. Of all 3d and 4d impurities only Pd remains non-magnetic since it approaches the atomic d^{10} configuration. The impurities with large d–moments even develop sizeable s–moments, as it naturally occurs for the atoms.

To our surprise we found that 5d impurities which up to now have not been experimentally investigated, show a similar strong magnetic behaviour as 4d ones [3]. For instance, Ta or W impurities should have local moments of 4–5 μ_B in the heavier metals. Even more, the calculations show that 2sp impurities like B, C or N might be magnetic in these exotic hosts. In a recent paper [4] we have extended these calculation to the divalent alkali–earth metals. The results are dominated by the large elementary volumes of the earth alkali metals and are similar to the above results for the alkali metals.

While the above calculations represent an important progress in understanding the magnetic properties of these exotic systems there are two problems which require substantial future work. Because of the large size difference between the impurity and the alkali hosts, one expects very large lattice relaxations, which are neglected in the present calculations. The second and even more important problem concerns the occurence of ionic configurations with atomic orbital moments which cannot be described in local density functional theory. I. Solovyev and one of the authors have therefore studied this problem within the LDA+U approach [5], based on a realistic calculation of the Hubbard U and exchange parameters. While we do not want to discuss this work in detail, it is fair to say that the LDA+U approach describes the localized configurations quite well, but with the calculated U–parameters it fails to describe the transition between itinerant and localized behaviour.

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The Screened Korringa-Kohn-Rostoker (KKR) Method

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(Jülich–Vienna Collaboration)

During the last decade, density-functional electronic-structure calculations have very substantially advanced the ability to understand and predict material properties from quantum-mechanical first principles. This progress can be attributed to the availability of powerful modern computers, but also to a large extent to the development of efficient numerical algorithms. A recent achievement in this respect is the discovery and development of the screened KKR method.

The use of screened structure constants is the main difference and advantage compared to the conventional, well-established method of Korringa, Kohn and Rostoker where the structure constants are complicated and difficult to obtain. Originally a phenomenological prescription for the screening was suggested and applied with success for surface electronic-structure calculations [1]. Afterwards it was demonstrated that the screening can be obtained by an exact transformation. Physically the screened structure constants can be understood as representing the Green function of a periodic system of strongly repulsive (e.g. square well) potentials. For low energies this Green function decreases exponentially in space and can easily be calculated for a finite cluster of repulsive potentials [2]. This gives a reformulation of the original KKR method into a first-principles tight-binding like form. The screening is most effective in the important energy range of the occupied electronic states. With respect to the spectroscopically important unoccupied states, recent tests have shown that even the empty-space density of states can accurately be obtained up to, at least, 40 eV where the extended states represent a severe test for any tight-binding like description.

From computational point of view, the method is well suited for large systems. It does not require eigenvalue determinations, but only matrix inversions for which efficient algorithms exist on sequential as well as on parallel computers. Due to the exponential decay of the structure constants, interactions beyond next-nearest-neighbor distances can be neglected which results in sparse matrices. For general three-dimensional problems the best algorithms must still be found, but clearly the computing effort increases more slowly with system size than in conventional methods where it grows with the cube of the number of electrons involved.

For surface and interface calculations the sparsity is straightforwardly exploited and leads to computing times which increase only linearly with system size, i.e. with the number of layers taken into account. Current applications include first-principles calculations of magnetic anisotropies for overlayer and interface problems (in Vienna) and the development of computer programs for interlayer exchange couplings (in Jülich) and for giant magneto resistance (in Dresden).

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Magneto-optical properties of magnetically ordered solids

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(Collaborative Activities within the HCM-network)

The dependence of optical properties of a solid on the polarization of light is a well-known phenomenon. Using the dielectric or, equivalently, the optical conductivity tensor to describe the optical response, this property can be traced back to its crystallographic structure, i.e. its symmetry. Loosely speaking, the lower the symmetry the more pronounced is the polarization dependence of the optical response in the solid. From this it is not astonishing that reducing the symmetry by imposing magnetic ordering on a solid gives rise to a dependence of the optical properties on the magnetic ordering, i.e. to magneto-optical effects. As for the crystallographically induced effects studying magneto-optical properties gives insight into the various microscopic consequences of magnetic ordering. In addition one can go the opposite way and control the optical properties by controlling the magnetic properties. These are the main reasons that magneto-optical effects are of such a great academic as well as industrial interest at the moment. The most prominent example for the latter is the magneto-optical Kerr-effect that has been known for more than 100 years. The Kerr-effect denotes the fact that light reflected by a magnetized sample changes its polarization upon reflection. This is made use of in data-storage and sensor technology or as an analytical tool to study surface magnetism.

Since the mentioned symmetry reduction has an impact only because of the spin-orbit coupling the theoretical description of magneto-optical effects has to account for magnetic ordering as well as relativistic effects at the same time. The approach to deal with this complex and challenging situation adopted by the collaborating groups in Bremen (Banhart), Bristol (Györffy), Budapest (Szunyogh), Daresbury (Durham, Guo, Temmerman), Keele (Strange), Munich (Ebert) and Wien (Weinberger), is based on the fully relativistic Dirac formalism for spin–polarized systems. During the last years corresponding band structure program packages have been developed, extended and refined using the conventional **k**–space as well as the more flexible multiple scattering formalism. Beside the magneto–optical Kerr–effect in the optical regime many new kind of spectroscopies in the X–ray regime have been studied using these codes. Here one has to mention the magnetic X–ray dichroism in absorption and emission, as well as the Faraday–effect in the X–ray regime. Recently corresponding studies of magnetic X–ray scattering have been performed. Application of the fully relativistic approach in combination with the Kubo–Greenwood–formalism gave access to the spontaneous magneto–resistance anisotropy and anomalous Hall resistivity. These galvano–magnetic effects are both of great importance for sensor technology. A further recent extension of the fully relativistic formalism allowed for a description of magnetic dichroism in core level and valence band photo-emission spectroscopy. A corresponding project to deal with this phenomenon in Auger electron spectroscopy was started last year.

Several of the above mentioned investigations pointed to a short-coming of the common theoretical basis: there is no feed-back of the spin-orbit induced electronic currents to the effective potentials. A way to overcome this problem meant to incorporate Brooks' orbital polarization approach into the multiple scattering formalism, which has recently been developed and successfully applied. A more satisfying way to achieve this would be to adopt current density functional theory. This route is explored at the moment in collaboration with Gross (Würzburg).

Finally one should emphasize that nearly all work mentioned above has been performed in close connection or collaboration with experimental groups. This is (at least partly) documented by the proceedings of a workshop on *Spin-Orbit Influenced Spectroscopies of Magnetic Solids* (published as Volume 466, in the Series "Lecture Notes in Physics", Eds.: H. Ebert and G. Schütz, Springer-Verlag, Berlin, 1996), that was attended to the same extent by theoretical and experimental workers in that field.

Magnetism of Transition–Metal Monolayers on Noble Metal Substrates

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(Jülich–Vienna Collaboration)

It is well known that almost all transition metals are nonmagnetic in their bulk phases. Among the 30 different transition metals only five are magnetic in the bulk: Ni and Co are ferromagnetic, Cr is antiferromagnetic, and Mn and Fe, depending on their bulk crystal structures, are ferromagnetic or antiferromagnetic. On the other hand, all isolated transition metal atoms show large magnetic moments which are governed by Hund's first rule. From this one may expect magnetic properties to depend drastically on the dimensionality or coordination number of the arrangement of transition metal atoms. Confining the atomic arrangement of transition metal atoms to monolayer films may lead to an enhancement of the magnetic moments within the monolayer and to new magnetic monolayers, made of transition metals, which are nonmagnetic in the bulk. Monolayer magnetism has been investigated experimentally in terms of transition metal monolayers on noble metal substrates, such as Ag, where the *d* bands lie about 3 eV below the Fermi energy and the *d*–*d* hybridization between a monolayer and the substrate is small.

Motivated by these arguments we have performed systematic *ab–initio* calculations for all 3*d*, 4*d*, and 5*d* transition metal monolayers on Ag(100) [1]. The calculations have been carried out using the FLAPW method in the film geometry within the density functional theory in the local spin-density approximation. They have revealed that practically all 3*d* monolayers are magnetic, even Ti and V, which are nonmagnetic in the bulk. The distribution of the magnitudes of the magnetic moments has turned out to be atomic–like with the maximum magnetic moment of about 4 μ_B at the center of the transition metal series (e.g. Mn in the 3*d* metal series).

To our great surprise we have also found magnetism in Tc, Ru, and Rh among the 4*d* metals, and Os and Ir among the 5*d* metals, associated with large magnetic moments between 1 μ_B and 2 μ_B. A closer look has revealed a strong deviation from simple atomic–like magnetism: The element with the largest moment among the 3*d*, 4*d*, and 5*d* monolayers has been shifted from Mn through Ru (isoelectronic to Fe) to Ir (isoelectronic to Co), respectively, while moving from 3*d*, through 4*d* to 5*d* metals. We have argued that this deviation resulted from a two-dimensional bandstructure effect causing the magnetism of 4*d* and 5*d* monolayers to be strongly dependent on the coordination number of the film.

We have investigated this aspect further by repeating the above calculations for 3*d*, 4*d*, and 5*d* transition metal monolayers, but on a Ag(111) surface [2,3]. A comparison between (100) and (111) orientations has elucidated the dependence of monolayer magnetism on a change of coordination number from 4 to 6 within the monolayer plane. The calculations for the (111) substrate have exhibited the same trend for the magnetic moments as has been found for the (100) substrate. Magnetism has been found for all 3*d* monolayers, for Ru and Rh among the 4*d* metals, and for Ir among the 5*d* metals. The element with the largest magnetic moment among each series has remained unchanged, but for 4*d* and 5*d* metals the size of the magnetic moments has changed drastically with the change of the coordination number: The reduction of the magnetic moment of Ir (85%, 5d element) has been larger than for Ru (30%, 4*d* element), while the magnetic moment of Mn (3*d* element) remained practically unchanged.

The calculations for (111) oriented substrates have been possible due to the development of a new FLAPW film code which is capable to treat any surface unit cell, and which does not make any explicit use of two(three)-dimensional inversion symmetry. However, despite this apparent progress, two questions remain unanswered and require future work: (i) For 4*d* and 5*d* transition metals one expects large spin-orbit interactions, which have been neglected in the present calculations. The large spin-orbit interaction may lead to a large magneto-crystalline anisotropy and a modification of the local moments [4]. (ii) For $3d$ monolayers on a (111) oriented substrate one also expects antiferromagnetic coupling of nearest neighbour atoms, leading to non-collinear magnetic phases.

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Theory of Pressure Induced Phase Transitions in the Cerium Pnictides

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(Aarhus–Daresbury–Karlsruhe Collaboration)

The Cerium Pnictides CeN, CeP, CeAs, CeSb and CeBi have peculiar properties as a function of applied hydrostatic pressure. At ambient conditions they all crystallize in the rocksalt (B1) crystal structure. With the exception of CeN the lattice constants indicate a trivalent nature of the Ce ions, corresponding to a configuration with one localized f-electron on each Ce atom. This is corroborated by the Curie-Weiss type susceptibility observed at elevated temperatures. In contrast, CeN is closer to a tetravalent Ce configuration corresponding to itinerant f-electrons and behaves as a Pauli enhanced paramagnet. Thus, CeN is similar to the collapsed α phase of pure cerium, where the cerium f-electron contributes actively to the cohesive properties, while the other Ce pnictides at ambient conditions are more similar to the γ phase of cerium. When pressure is applied, discontinuous structural phase transitions occur in all the cerium pnictides, with the exception of CeN. In CeP a peculiar *isostructural* transition is observed at a pressure of $P_1 \sim 90$ kbar accompanied by a volume collapse of $\Delta V_1 \sim 3\%$. This transition is similar in appearance to the isostructural $\alpha \leftrightarrow \gamma$ phase transition in cerium metal, and is usually attributed to a change from (predominantly) trivalent to (predominantly) tetravalent behavior of the cerium ions. At a higher pressure of $P_2 \sim 150$ kbar a second transition to the CsCl (B2) structure is observed, with a volume collapse of $\Delta V_2 \sim 10\%$. In CeAs, a single B1→B2 phase transition occurs at a pressure of $P \sim 145$ kbar with a volume collapse of $\Delta V \sim 11\%$. While some authors have claimed that no substantial change in Ce valency occurs at the transition, others conclude a significant change. In CeSb and CeBi a high pressure tetragonal phase is observed, at $P \sim 85$ kbar and $P \sim 90$ kbar, respectively, with volume collapses of $\Delta V \sim 11\%$ and $\Delta V \sim 9\%$, respectively. The tetragonal phase may be viewed as a uniaxial compression of the CsCl structure with a c/a ratio of 0.82 in CeSb and 0.84 in CeBi. In both cases the Ce ions are considered to remain trivalent across the phase transition.

In the present work a systematic theoretical investigation of the Ce pnictides has been undertaken. The electronic structure of the cerium pnictides was calculated with the self-interaction corrected local-spin density (SIC-LSD) approximation implemented with the LMTO method. This scheme offers the possibility of describing the Ce f-electrons as either localized or delocalized. By comparing calculations in different structures and different treatments of the f-electrons, all the phase transitions observed in the cerium pnictides are reproduced with excellent quantitative agreement, as demonstrated in Table I. The present calculations find the CeAs high pressure phase to be described with delocalized f-electrons. The isostructural B1(loc)→B1(deloc) transition is only barely missed, but the calculations do not offer a possibilty of a B1(loc)→B2(loc) transition.

The observed trends in the crystal structures of the cerium pnictides can be explained in a simple way: With increasing Z of the ligand, the specific volume (at zero pressure) increases while the ionicity of the compound decreases. The delocalization of Ce f-electrons is less favorable at large specific volumes (since interatomic hopping matrix elements are small), while the CsCl structure is favored over the NaCl structure with decreasing ionicity. The tetragonal structure observed at high pressure in CeSb and CeBi is almost degenerate with the undistorted CsCl structure.

The magnetic properties of the cerium pnictides are quite complicated with several antiferromagnetically ordered phases and phase transitions at low temperatures. The resistivities of the CeP, CeAS, CeSb and CeBi systems show semimetallic or small–gap semiconductive characteristics at ambient conditions. A negative slope of the resistivity as a function of temperatures indicates that Kondo type screening occurs in the ground state of the cerium pnictides. Calculations with the SIC-LSD method for CeP in the AFI structure confirm this semimetallic behaviour.

The exact ground states of the cerium pnictides are bound to be much more complicated

Compound	Character	P_t/kbar		$\Delta V/V_0$	
		exp.	theo.	exp.	theo.
CeP	B1(loc)→B1(deloc)	90	71	3%	8%
CeP	B1(deloc)→B2(deloc)	150	113	10%	12%
CeAs	B1(loc)→B2(deloc)	145	114	11%	18%
CeSb	B1(loc)→tet(loc)	85	70	10%	11%
CeSb	tet(loc)→tet(deloc)	-	250	-	4%
CeBi	B1(loc)→tet(loc)	90	88	9%	9%

Table 1: Experimental and theoretical phase transition pressures and volume collapses in the cerium pnictides.

than the simple picture offered by the SIC-LSD method, which still, like the LDA, describes the system in terms of a single Slater determinant. The good agreement between the SIC-LSD theory and experiments shows, however, that the method is accurate enough to reproduce the cohesive properties of correlated electron materials. In particular, the energy of localization, which in the SIC-LSD is given as the self-interaction correction of the localized f-electron, has the correct magnitude. In CeP this energy is ~ -65 mRy, which is countered by the 'band-formation energy' to produce the delicate balance between the trivalent and tetravalent configurations. It remains a challenge for the coming years to extend the accuracy of the present calculational scheme and to augment the formalism in such a way that other physical properties may be considered, like e.g. photoemission experiments.

Rennes[1] - Zürich[2] collaboration on the electronic and dynamical properties of molecular charge-transfer compounds

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P. E. Blöchl *(IBM Zürich, Switzerland)*[2]

Charge transfer salts exhibit a dazzling variety of different structural and electronic phase transition. Members of this class are superconductors, ferroelectrics, antiferro- and ferrimagnets, and exhibit Peierls and neutral to ionic transitions. Close to the transition spin and charge solitons have been observed. The transitions can be driven by pressure, temperature, photoirradiation etc. Charge transfer salts are molecular crystals with typicaly two types of large organic molecules assembled in low dimensional structures. Thus they exhibit features ranging from zero to three dimensions. These structures are an ideal ground for fundamental studies, which may help in the understanding of other low dimensional and correlated materials.

Despite active research over several decades, a detailed microscopic understanding of these materials is still elusive. The structural complexity has prohibited accurate first-principles calculations in the past. Only recently this situation changed owing to new simulation techniques such as the Projector Augmented Wave method developed at the IBM Zürich Research Laboratory.

In our quest to obtaining a global understanding of these materials and their transitions, we have selected the prototypical material for neutral to ionic transitions, namely tetrathiafulvalene-chloranil or short TTF-CA. So far we have studied the vibrational spectra depending on charge state of chloranil in order to make contact with experiments that deduce the ionicity of the crystal from the measured i.r. and Raman spectra. This work will soon be published in Physical Review. Currently we are proceeding to deriving the parameters that are essential for the transition. We have so far evaluated ionization energies and electron affinities, the intra– and inter–molecular Coulomb interaction, spin splitting parameter, hopping integrals and as of writing this article we are in the process to extract the relevant phonon interactions. Once the model is completed, it will allow us to *derive* a consistent description, from which the complex nonlinear exitations and phase transitions can be simulated and elucidated.

The expertise gained in this study is expected to be useful to understand materials of technological interest such as organic magnets, superconductors, and dyes, conducting polymers and materials for light emmitting diodes.

This collaboration has been initiated in 1994, by a joint project between IBM-Zürich and the University of Rennes, and has been partially funded by the Psik-network. This project has started with the training of C. Katan (young researcher in Rennes) in the CP-PAW method, to reach a perfect knowledge of all the possibilities of the code. During the course of this collaboration, C. Katan spent in total 2.5 months at IBM-Zürich research Laboratory.

Highlights of the collaboration between T.U. Vienna and IBM Zurich Research Laboratory

Adsorption of water and methanol in zeolites

E. Nusterer, K. Schwarz *(Technical University Vienna)*
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Zeolites are microporous aluminasilicates, which are important catalysts in petrochemistry used for cracking and the production of fine chemicals. The catalytic function of zeolites rests with steric hindrance inside the pores and cages with catalytic centers distributed over the internal surface of zeolites. The most common catalytic centers are acid sites, namely AlOH fragments, which replace a SiO fragment of the framework. Despite the critical importance of the interaction of polar molecules with acid site centers for the catalytic reactions, the adsorption properties of even simple molecules such as water and methanol have not yet been resolved.

The most direct experimental information is available through ir spectroscopy. However, owing to the unusual bonding arrangements in zeolites, the interpretation of these results depends largely on their comparison with theoretical calculations. Previous quantum chemical calculations have been limited to small clusters and the inability to investigate finite temperature behavior, and hence have been unable to reproduce the experimental spectra.

Therefore, we have performed finite-temperature simulations of methanol and water in a zeolite called sodalite at low and high coverages (E. Nusterer, P.E. Blöchl and K. Schwarz, Angew. Chem. 1996 in press). Our approach, the projector augmented wave method combined with the ab-initio molecular dynamics scheme of Car and Parrinello, allows periodic zeolite crystals to be studied and provides access to finite-temperature dynamics. Simulations of methanol at low coverages, i.e. one methanol molecule for every second cage of sodalite, have been performed for 20 psec. The calculations reproduce all main features related to hydrogen bonds observed by experiment, but also provide us with a microscopic picture of the structure and dynamics. We observed that methanol forms one very strong hydrogen bond with the acid site, whereas a second hydrogen bond can exchange between several hydrogen bond acceptors of the framework. One of the two types of structures observed has not yet been proposed because it involves framework oxygen atoms that are too distant to have been included in previous quantum chemical calculations.

At high coverages, however, the picture changes qualitatively (E. Nusterer, P.E. Blöchl and K. Schwarz, submitted to Chem. Phys. Lett.) Although no protonation of water and methanol have been observed when only one methanol was adsorbed per acid site, two molecules already result in almost perfect protonation and in the formation of hydroxonium-like structure adsorbed via hydrogen bonds to the zeolite framework. This finding has important consequences on the catalytic reactions in zeolites: reactions typically performed at larger coverages therefore qualitatively resemble those in a similar acid-catalyzed reaction in the liquid, except for a dramatically increased proton concentration. The structural changes upon increasing coverage is reflected in a qualitative change of the measured adsorption spectra, which are well reproduced by our simulations.

Not only are the changes of the spectra upon increasing partial pressure well reproduced, but also selective deuteration experiments are in line with our predictions, lending strong support to our model of the adsorption of small polar molecules in zeolites.

Structure and vibrational properties of metallocenes

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In preparation of investigations of catalytic reactions using transition metalorganic complexes we have investigated structural and dynamical studies of metallocenes such as ferrocene (P. Margl, K. Schwarz and P.E. Blöchl, J. Chem. Phys. 100, 8194 (1994)) and beryllocene (P. Margl, K. Schwarz and P.E. Blöchl, J. Am. Chem. Soc. 116, 11177 (1994), *ibid* J. Chem. Phys. 103, 683 (1995). Ferrocene is a sandwich compound with an Fe(II) ion sandwiched between two aromatic cyclopentadienyl rings $C_5H_5^-$. This molecule is a classical test system and has been studied extensively using quantum chemical methods because its bonding is severely influenced by electronic correlations not present in the Hartree–Fock approach. On the other hand its size is small enough to allow accurate correlated methods to be applied. The trajectories from finite temperature simulations have been analyzed to obtain the vibrational modes and frequencies using an approach inspired by previous work of Kohanoff and Parrinello. A comparison reveals deviations of the order of a few percent in the vibrational spectrum. Furthermore our work has resulted in a reassignment of the experimental absorption spectra. The dynamical properties of a related molecule, which in contrast to the rather stable ferrocene shows fluxional behavior, have been elucidated with the present approach. Thus we have successfully tested the Car–Parrinello projector augmented wave method for two limiting cases of organometallic behavior.

These calculations have opened the door for investigations of organometallic catalytic reaction mechanisms performed to date. They include the enantioselective allylic amination using Pd(II) catalysts with bidentate P-N,ferrocenyl ligands (P.E. Blöchl and A. Togni, submitted to J. Am. Chem. Soc.), polymerization reactions using zirconocene catalysts (P. Margl, J.C.W. Lohrenz, T. Ziegler and P.E. Blöchl, submitted to J. Am. Chem. Soc.) and to carbonylation of methane using an Rh catalyst (P. Margl, T. Ziegler and P.E. Blöchl, J. Am. Chem. Soc. 117, 12625 (1995), *ibid* submitted).

About the collaboration between T.U. Vienna and IBM Zurich Research Laboratory

The collaboration between the group of Prof. K. Schwarz at the Technical University of Vienna and Dr. P.E. Blöchl at the IBM Zurich Research Laboratory has been very active. This has included regular, extended visits of Ph.D. students of Prof. K. Schwarz, namely E. Nusterer, P. Margl and J. Sarnthein, in Zurich, one extended stay of P.E. Blöchl at the Technical University of Vienna, and several short visits of the project coordinators.