

## $\Psi_k$ Network

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

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## Editorial

Please note that for convenience in this newsletter we have changed the LaTeX '*documentstyle*' from '[12pt]' to '[11pt]'.

The **Editorial** is followed by the section **News from the Network** where we summarize on the impact of workshops, organized by the Network in the past two years, on research of the participants and future science in different universities and different countries.

In the section **News from the Working Groups** readers will find reports on recent collaborative visits and workshops.

Straight after the reports there are announcements of forthcoming workshops in Bristol, Halle and Strasbourg. All are co-organized by the Network.

In this *Newsletter* readers can also find the **3rd Circular of the Network Conference**. For convenience it is placed at the end of the *Newsletter*, where we have also attached *an application form* to receive financial support for attending the Conference, and *an abstract form* for submitting abstracts of contributions to the Conference. Please note that the *hotel reservation cards*, mentioned in the circular, are not available via e-mail. More information on the **Conference** is available from the organizers whose coordinates are given in the 3rd circular. The **3rd Circular** and all other relevant information concerning the **Network Conference** are also available on **WWW** at

<http://radix2.mpi-stuttgart.mpg.de/hcm.html>.

Announcements of available positions follow the announcements of workshops. **Abstracts** section is as usually placed after the job announcements.

In the section **Presenting Other Initiatives** there is an article on the activity of CECAM by *Stefano Baroni*, the present director of CECAM.

In the **Highlight of the Month** section readers will find an article by *L.M. Sandratskii and J. Kübler (Darmstadt)* on '**Non-collinear magnetism: effects of symmetry and relativity**'.

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

The above contains pointers to several other nodes: *O.K. Andersen (Stuttgart)* which also includes information on the **Network Conference**, *P. Blöchl (IBM, Zürich)*, *M. Gillan (Keele)*,

*E.K.U. Gross (Univ. Wurzburg), B.L. Györfly (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.

	<b>function</b>
<b>psik-coord@daresbury.ac.uk</b>	<b>messages to the coordinator &amp; newsletter</b>
<b>psik-management@daresbury.ac.uk</b>	<b>messages to the NMB</b>
<b>psik-network@daresbury.ac.uk</b>	<b>messages to the whole Network</b>

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

# News from the Network

## Impact of the Network on Future Science

To be able to assess the impact of the Network on research of the community and future science, we have monitored three of the many workshops that have been organized by the Network in the past two years. One of them was a general workshop on *Improved Density Functionals* in Aarhus, and the other two were '*Hands-on*' *Molecular Dynamics and TB-LMTO Computer Codes* workshops, in Berlin and Stuttgart, respectively. We have contacted all the participants of these workshops by e-mail, asking for their opinion on the usefulness of the workshops for their own research and research of the groups in which they work. On average over 60% have responded; some participants have since changed place of their employment and have not contacted us. Below we summarize the response that has been received.

- **Improved Density Functionals Workshop** took place in Aarhus (Denmark) on 18–19 June 1994. It was organized by A. Svane (Aarhus). The workshop had 44 participants; 40 participants were from EU or associated countries, and four from Eastern Europe. Response has been received from 29 participants, all of whom considered the workshop extremely useful, and one of the best they had attended. The most valued aspect of the workshop, stressed mostly by younger participants, was the general overview of the field that it presented, allowing one to decide which of the currently available improved functionals should be best used in one's research. Some stressed that the workshop allowed them to gain deeper understanding of relations between various improved functionals like self-interaction corrections, orbital polarisation and gradient corrections. Some gained reassurance that their line of research is worthwhile to pursue. Many, mostly already well established scientists, got an inspiration for new directions in their research, got new ideas, adapted new approaches presented at the workshop and/or started new collaborations. Five new collaborations were started at the workshop and have continued fruitfully ever since. Also, a few papers have been published acknowledging benefits from the Network owing to the workshop.
- **Hands-on Molecular Dynamics Code Workshop** was held in Berlin on 3–7 October 1994. It was organized by J.L. Martins (Lisbon) and the group of M. Scheffler at the FHI in Berlin. The workshop had 18 participants; 12 were from EU or associated countries, and six from outside. Thirteen participants have responded to us with their opinions and assessment. Out of those who responded, eight have used the code, some very extensively, after the workshop. A few papers published after the workshop have acknowledged the Network indirectly, through the FHI Berlin group. Five participants have not made use of the code after the workshop, but have used the knowledge acquired at the workshop to develop their own codes, sometimes taking over parts of the Berlin code. All participants valued the well structured programme of the workshop and a good balance

between the practical aspects of running the large *ab-initio* code and the underlying theory on electronic structure methods and their applications. The acquired ability to run a large first-principles code, which allowed some participants' groups to move to the field of *ab-initio* calculations, was extremely appreciated.

- **Hands-on TB-LMTO Code Workshop** took place in Stuttgart on 24-28 October 1994. It was organized by the group of O.K. Andersen at the Max-Planck-Institute in Stuttgart. This workshop had 15 participants; 13 were from EU or associated countries, and two were from Eastern Europe. At the end of the workshop a questionnaire on the usefulness of the workshop was distributed to all participants. In general, the workshop was well received but some of the participants expected more lectures on the theory of the LMTO method, than was given at the workshop. To our recent survey we have received a response from 10 participants, either directly or through the organizers. Seven of the participants use the code; one of the seven works on further development of the code, another has already published two papers on the basis of the code, acknowledging the benefits from the Network through the workshop. One of the participants has been using the older version of the TB-LMTO code, but expects that he or other members of the group will use the code in future. After the workshop one participant has decided to use the FP-LAPW WIEN95 code, instead of the TB-LMTO, as a basis for his own development; a decision that was possible owing to the attendance of the workshop. Nearly all outside EU participants had a problem with installation of the code on their respective computers, due to insufficient compute memory, however even they have found the workshop and code useful for their own developments of computer codes, and may in future use the code subject to better computing facilities.

## Report on the collaborative visit of J.E. Inglesfield (University of Wales Cardiff) to University of Nijmegen 14–18 February, 1996

On 15th–16th February I visited the Electronic Structure of Materials group in Nijmegen (where I worked until September last year) to collaborate with Jeroen van Hoof on the development of the embedding method for surfaces and interfaces, and to discuss magnetic systems with Rob de Groot, Peter van Gelderen and Theo Rasing.

Jeroen van Hoof has further developed and implemented a new embedding method based on a paper published several years ago (Crampin, Van Hoof, Nekovee and Inglesfield, *J. Phys.: Condens. Matter* **4**, 1475 (1992)), in which the bulk, interfaces and surfaces are all treated on the same footing. The material is “grown” layer by layer, and the embedding potential transferred through successive layers using Green function techniques. Jeroen uses LAPW basis functions in a full potential framework, and the computer programs which he has developed are now at the production stage. On my visit we discussed the inevitable problems which arise in any large new program.

Peter van Gelderen, with Simon Crampin and myself, completed last year a student project on quantum well states, and recently we have been looking at the effect of interface magnetic moments on magnetization-induced second harmonic generation with Theo Rasing. Theo Rasing’s experimental group in Nijmegen has shown large magnetic effects in second harmonic generation (an intrinsically surface and interface sensitive technique), in particular thickness-dependent effects in Co/Cu(001) and Cu/Co(001) systems. These we have been trying to explain in terms of a parametrized model for the magnetization-dependent non-linear susceptibility, and a paper has been written on this (“Effect of interface magnetic moments and quantum well states on magnetization induced second harmonic generation”, submitted to *Phys. Rev. B*; abstract included in this Newsletter).

(J.E. Inglesfield)

**Report on the collaborative visit of Peter Vansant (Antwerp) to  
Lisbon  
10–13 March, 1996**

Peter Vansant from the Antwerp node of Vic Van Doren and Piet Van Camp visited Jose Luis Martins in Lisbon from March 10 to 13 in the framework of a collaboration on ternary calcium nitrides. The objective of the visit was to apply molecular dynamics and conjugate gradient techniques to the optimization of the structural parameters of the perovskite based materials. As the calcium octahedra are tilted the number of internal structural parameters is quite high, requiring efficient structure optimization techniques.

(J.L. Martins)

# Report on the Bond Order Potential Workshop

## 18–19 March, 1996

The second Bond Order Potential (BOP) workshop has just concluded. It was held in the Department of Materials at the University of Oxford, and received financial support from the EPSRC, through CCP9, for participants from the UK, and from the Naval Research Laboratory for participants from the USA.

The aims of the Workshop are described below.

*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) were presented. Bond-order potentials 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 were also described and their relative merits discussed with reference to particular modelling problems.*

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

The workshop was well attended, there were 55 registered participants from a number of countries, including the UK, the USA, Sweden, France, Austria and Greece. The feedback received so far has been positive.

The following points have become apparent as a result of the workshop:

1. There is a need for methods for evaluating energies and forces for molecular dynamics simulations that are more accurate than the conventional empirical potential models, but are still computationally highly efficient. Further, clear schemes for working with systems composed of more than one type of material are needed (e.g. metal/ceramic interfaces). Tight binding is viewed as a very promising way forward.
2. Clear schemes for fitting tight binding parameters are needed. The OXON package offers some help with fitting, but a completely defined general procedure has yet to be worked out.

(Andrew Horsfield)



# INTERNATIONAL WORKSHOP ON THE BOGOLIUBOV-de GENNES EQUATIONS FOR SUPERCONDUCTORS

*Sponsored by: CCP9 and EU-HCM  $\psi_k$ -Network*

*Organised by: B.L. Györfly (b.gyorffy@bristol.ac.uk)*

**H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue,  
Bristol, BS8 1TL, UK**

*March 30, Saturday, 10:00am–March 31, Sunday, 2:00pm*

This workshop is the third in the Bogoliubov–de Gennes series of workshops. This year the following speakers and talks are planned. Further details are available from Professor B.L. Györfly at the above e-mail address, or Kevin Duncan (secretary of the Workshop) at: kevin.duncan@bris.ac.uk.

## PROGRAMME:

Stefan Kurth ( <i>Antwerp</i> )	<b>Local Density Approximation for Superconductors</b>
Walter M. Temmerman ( <i>Daresbury</i> )	<b>Quasi-particle Spectra of High Temperature Suprconductors</b>
Balazs L. Györfly ( <i>Bristol</i> )	<b>A semi-calssical Theory for Superconductors</b>
Jonathan Robins ( <i>Bristol</i> )	<b>Semi-classical Quatization: The Modern View</b>
Colin Lambert ( <i>Lancaster</i> )	<b>Superconducting Nano Structures</b>
Klaus Capelle ( <i>Würzburg</i> )	<b>Dichroism in Superconductors</b>
James Annett ( <i>Bristol</i> )	<b>The evidence for d-wave pairing in High Temperature Superconductors</b>
A.S. Alexandrov ( <i>Loughborough</i> )	<b>Bose-Einstein Condensation of Charged Particles in a Magnetic Field</b>
Grzegorz Litak ( <i>Lublin</i> )	<b>Percolating Superconductivity</b>
John Matthias ( <i>Exeter</i> )	<b>Quasiparticle scattering in Superfluid Helium 4</b>
Martin Lüders ( <i>Würzburg</i> )	<b>The decoupling scheme for the Bogolubov-de Gennes equation and symmetry considerations for the gap equation</b>

# Workshop on Fe/Cr interface magnetism

Satellite Meeting of the Symposium  
of the E-MRS Spring Meeting '96 on:  
**Magnetic Ultrathin Films, Multilayers and Surfaces**  
(Strasbourg, Congress Center, 4-7 June 1996)

Workshop partially supported by the EU-HCM - network:  
**AB-INITIO (FROM ELECTRONIC STRUCTURE)  
CALCULATION OF COMPLEX PROCESSES IN MATERIALS**

This workshop will be held from **Sunday the 2nd of June at 2pm to Monday the 3rd of June at 6pm**. It will consist of scheduled speakers followed by discussions in an informal atmosphere. The meeting will take place at the Institut de Physique Chimie des Matériaux de **Strasbourg** (IPCMS) located 5 kilometers from the Congress Center, the place of the E-MRS Spring Meeting '96.

The widely studied Fe/Cr system presents several intriguing phenomena related not only to interdiffusion, roughness and growth but also to the complicated magnetism of the Cr itself and especially the modification of the spin density wave (SDW) according to the Cr thickness. Despite the progress which has recently been made it is now clear that there remain many unresolved questions following the recent reports of new findings connected with the antiferromagnetism of the Cr and the atomic level structure of the Fe/Cr interface. A focused discussion meeting of such issues and controversies is both timely and appropriate. It is also appropriate to relate the present work to studies of bulk Cr.

## Scope & Topics

- + structural characterization, growth mode
- + layer dependent magnetic moment distribution, anisotropy, roughness
- + GMR, interlayer coupling
- + SDW, temperature effects, bulk Cr

## Preliminary list of contributors and participants (updated 10 March 1996)

A. Berger (La Jolla), S. Blügel (Juelich), P. Bruno (Orsay), JAC Bland (Cambridge), D. E. Buerger (Basel), B. Carrière, M. Freyss, F. Scheurer, D. Soeffler (Strasbourg), B. Coqblin (Orsay), A. Davies, M. Stiles (NIST), P. H. Dederichs, K. Wildberger (Juelich), S. Demokritov (Kaiserslautern), J. Dorantes-Davila (San-Luis Potosi), V. Dupuis (Lyon), P. Gruenberg (Juelich), H. Hasegawa (Tokyo), B. Heinrich (Burnaby), F. Himpsel (Madison), H. J. Hug (Basel), Y. Kawazoe (Tohoku), E. Kisker, D. Knabben, F. Hillebrecht (Duesseldorf), Th. Kleinefeld (Duisburg), N. Kulikov (Troitsk), J. Meersschaut, M. Rots (Leuven), I. Mertig (Dresden), S. Miethaner, G. Bayreuther (Regensburg), D. L. Mills (Irvine), S. Mirbt (Uppsala), S. N. Okuno (Kawasaki), S.S.P. Parkin (San Jose), F. Petroff and A. Fert (Orsay), M. Piecuch (Nancy), J. Pflaum, D. Kurowski (Bochum), T. Rasing (Nijmegen), G. Reiss (Dresden), C. M. Schmidt (Basel), I. K. Schuller (La Jolla), W. Temmerman (Daresbury), V. V. Ustinov (Ekaterinburg), V. Uzdin (St-Petersburg), A. Vega (Valladolid), H. Zabel, A. Schreyer, P. Boedeker (Bochum),

Attention: the number of participants will be limited to 65.

## Symposium organizers

Hugues Dreyse  
IPCMS-GEMME  
BP 20 CR  
67037 Strasbourg Cedex  
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*1st Announcement*

## Workshop MNS96

# Magnetic Nanostructures on Metal and Semiconductor Surfaces - Theory and Experiment -

*Supported in part by the EU HCM  $\Psi_k$ -Network on*

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

- Date** : 20.05.96 - 21.05.96
- Location** : FB Physik, Martin-Luther-Universität Halle-Wittenberg, Halle  
MPI für Mikrostrukturforschung Halle, Halle
- Organization** : Dr. W. Hergert, FB Physik, Universität Halle  
Prof.Dr. Kirschner, MPI für Mikrostrukturforschung Halle
- Schedule** : 07.4.96 - registration, offer of contributions  
18.4.96 - 2nd announcement, preliminary programme  
05.5.96 - deadline for registration and final programme
- Contacts** : Dr. Wolfram Hergert  
Department of Physics  
Martin-Luther-University Halle-Wittenberg  
**D-06099 HALLE**
- Email** : hergert@physik.uni-halle.d400.de

### Aim

A lot of theoretical and experimental work has been done in the last few years to study low dimensional metallic systems. One of the challenging problems is the magnetism in low dimensional metallic structures consisting of materials which are non-magnetic in the bulk.

Recently the interest in the study of the magnetic properties of free and supported clusters has increased. New methods are developed to create in a defined way metallic clusters on metallic surfaces. The measurement of the electronic and magnetic properties of such metallic nanostructures is a very complicated problem.

The aim of the workshop is to bring together theoreticians and experimentalists, working in this field, to discuss the state of the art in calculating magnetic properties of free and supported metallic clusters as well as the present status of experimental studies of such nanostructures. The workshop is expected both to help reserchers in finding new ideas for their future work and to possibly start new colaborations between theoreticians and experimentalists.

### Details of Organization

- We want to organize cheap accomodations in Halle. Details will be given in the next announcement. There will be no workshop fee. The workshop will be held in the MPI für Mikrostrukturforschung and the Department of Physics of the University.
- We want to have enough time during this workshop for intensive **discussions**. Therefore the number of talks will be limited. Up to now we have not planned to organize a poster session.

- To use the two days most effectively the arrival should be planned for Sunday. We do not want to start too late on Monday morning. The participants are free to depart either on Tuesday evening or on Wednesday.
- Members of the Network may apply for financial support.
- Please use E-mail to communicate with the organizer (Subject: MNS96)

**Colleagues already interested in our project are:**

- Prof. K. Kern, EPF Lausanne, Switzerland
- Prof. P. Jena, Virginia Commonwealth University, Richmond, U.S.A.
- Prof. P.H. Dederichs, IFF Forschungsanlage Jülich, Germany
- Prof. H. Dreyssé, IPCMS Strasbourg, France
- Prof. L.C. Balbás, University of Valladolid, Spain

(Dr. W. Hergert)

*Announcement*

**Postdoctoral Research Assistant in "Electronic  
Structure Calculations"**

*University of Bristol*

*Department of Physics*

Applications are invited to work on the flag-ship project of CCP9 (Computational Collaborative Project 9 of the EPSRC) involving calculations of surface magnetic anisotropy from first principles. Experience with LMTO and KKR band theory methods would be desirable.

The successful candidate will be member of the Bristol Theory Group but the work will entail collaboration with groups in the UK and Europe.

**Salary range: 14,317–16,628 GBP p.a.**

Informal enquires may be directed to Professor B.L. Györffy, Department of Physics on +44-(0)117-928 8704 or email B.Gyorffy@Bristol.ac.uk.

For further details telephone +44-(0)117-925 6450 (ansaphone after 5pm), minicom +44-(0)117-928 8894, e-mail Recruitment@bris.ac.uk, or write to the Personnel Office (EO), University of Bristol, Senate House, Bristol, BS8 1TH, quoting reference E217.

**The closing date for applications is 1st May 1996.**

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An International Centre for Education and Research

## *Announcement*

### **Postdoctoral Positions for Young EU Nationals**

An EU-funded Training and Mobility Research (TMR) Network on Interface Magnetism has positions\* for 7 young (less than 35 years) EU nationals for the following projects:

- Interlayer Exchange Coupling (Coordinator: B.L. Gyorffy, Bristol, UK)
- Spin-polarised Spectroscopies (Coordinator: W.M. Temmerman, Daresbury, UK)
- Tight Binding KKR Green's Function Methods (Coordinator: P. Dederichs, Juelich, Germany)
- Real Space Tight Binding LMTO Methods (Coordinator: H. Dreysse, Strasbourg, France)
- Spin-polarised Spectroscopies (Coordinator: P. Weinberger, Vienna, Austria)
- Giant Magnetoresistance (Coordinator: P. Kelly, Eindhoven, Netherlands)
- Magnetic Anisotropy and Surface Structure (Coordinator: B. Johansson, Uppsala, Sweden)

The Network consists of six flagship projects, which we consider as the most important and highly challenging ones in *ab-initio* electronic structure calculations of magnetic properties. Four of the flagship projects include studies of the most recent discoveries of interlayer coupling, giant magnetoresistance and magnetic X-ray dichroism. The other two projects concern the implementation of new technical developments in electronic structure calculations (i.e. screened structure constants) to construct a new generation of codes able to deal with larger systems. Consequently we will be able to perform *ab-initio* studies of interlayer coupling, giant magnetoresistance, magnetic anisotropies and surface structures for realistic systems, larger than ever studied before. In particular we want also to study the interrelation between these properties. Moreover we want to carefully compare the details of our calculations against spectroscopic data. Each flagship project will be spearheaded by a post-doc, the only exception being the spectroscopy project which has 2 post-docs associated because of the interaction with synchrotron communities.

Additional information may be obtained from:

Peter Dederichs, e-mail: L.Gerken@kfa-juelich.de, Tel.: +49-2461-614351, Fax: +49-2461-612620  
Walter Temmerman, e-mail: w.m.temmerman@dl.ac.uk, Tel.: +44-1925-603227, Fax: +44-1925-603634

\* subject to the satisfactory conclusion of contract negotiations and financial procedures with the European Commission. Only nationals of EU Member States different from the country where the project is located are eligible.

# ANNOUNCEMENT

## POST-DOCTORAL POSITION

Philips Research Laboratories Eindhoven, The Netherlands

### Interface Magnetism: Giant Magnetoresistance

Candidates are invited to apply for a two-year post-doctoral position\* to work on the theory of Giant Magnetoresistance (GMR) with the Dutch partners of the Network *Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers* sponsored by the European Union's Training and Mobility of Researchers programme.

The aim of the theoretical collaboration between Philips Research Laboratories, Eindhoven (P.J. Kelly) and Delft University of Technology (G.E.W. Bauer) is to bridge the gap between phenomenological models of GMR and realistic ab-initio descriptions of the electronic structure in layered magnetic materials. The NL post-doc will extend our studies of transport in mesoscopic systems [PRL74(1995)586] using the Landauer scattering formalism, making use of suitable electronic structure codes being developed within the Network. The post-doc will collaborate closely with experimentalists at Delft Institute of Microelectronics and Submicrontechnology (DIMES), where the effort is concentrated on ballistic point contacts in the nanometer regime, as well as at Eindhoven, where the experimental work on the GMR forms part of an ESPRIT project coordinated by Philips. The research position is expected to be based in Eindhoven and maintain intensive contact with Delft.

Applications should be sent to  
Dr. P.J. Kelly,  
Philips Research Laboratories Eindhoven,  
Prof. Holstlaan 4,  
5656 AA Eindhoven,  
The Netherlands

Additional information may be obtained from:

kelly@natlab.research.philips.com, Tel.: +31-40-2742676, Fax: +31-40-2743365  
bauer@duttnto.tn.tudelft.nl, Tel.: +31-15-2784719, Fax: +31-40-2781203

\* subject to the satisfactory conclusion of contract negotiations and financial procedures with the European Commission. Only nationals of Member States or Associated States of the EU (but not the Netherlands) are eligible for the position allocated to the Dutch node.



*Announcement*

**Postdoctoral Position in "Electronic Structure  
Theory"**

*University of Missouri, Columbia, USA*

A post-doc position in computational condensed matter physics (electronic structure of solids) is available beginning September 1, 1996 in the Department of Physics, University of Missouri, to work in collaboration with Prof. S. Satpathy on the electronic structure of magnetic materials. The successful candidate should have significant experience in density-functional calculations of the electronic structure of solids using the LMTO or other methods. The appointment will be for one year initially and may be extended for another year subject to the availability of funding.

Interested candidates should send a resume including names of references and recommendation letters either by e-mail to:

**satpathy@agni.physics.missouri.edu**

or by regular mail to:

**S. Satpathy, Max-Planck-Institut, Heisenbergstr. 1,  
D-70569 Stuttgart, Germany** (sabbatical address),

AS SOON AS POSSIBLE.

# Electronic structure and magnetic properties of random alloys: fully relativistic spin-polarized linear muffin-tin orbital method

A.B. Shick<sup>a,b</sup>, V. Drchal<sup>a,c</sup>, J. Kudrnovský<sup>a,c</sup> and P. Weinberger<sup>c</sup>

<sup>a</sup> *Institute of Physics, Academy of Sciences of the Czech Republic,  
Na Slovance 2, CZ-180 40 Praha 8, Czech Republic*

<sup>b</sup> *Institute of Solid State Chemistry, Ural Division of RAS,  
GSP-145 Pervomaiskaia 91, Ekaterinburg, Russia*

<sup>c</sup> *Institute for Technical Electrochemistry, Technical University,  
Getreidemarkt 9, A-1060 Vienna, Austria*

## Abstract

A Green's function method is developed to calculate the electronic and magnetic properties of random alloys containing heavy elements. Based on the local spin density approximation, the all-electron spin-polarized version of the fully-relativistic linear muffin-tin orbital method in the tight-binding representation is used to describe disorder within the coherent potential approximation. The method is first tested on ferromagnetic 3d metals (Fe, Co, Ni) and then applied to study the electronic and magnetic properties of the fcc alloy systems  $\text{Co}_{50}\text{Ni}_{50}$  and  $\text{Co}_{50}\text{Pt}_{50}$ .

(submitted to Phys. Rev. B)

Manuscripts available from: [pw@eecs1.tuwien.ac.at](mailto:pw@eecs1.tuwien.ac.at)

# The *TB-LMTO method* and its relation to the *Screened KKR method* \*)

P. Weinberger<sup>1,2)</sup>, I. Turek<sup>1,3)</sup> and L. Szunyogh<sup>1,4)</sup>

<sup>1)</sup> *Center for Computational Materials Science, Vienna, Austria*

<sup>2)</sup> *Institute of Technical Electrochemistry,  
Technical University Vienna, Austria*

## Abstract

The main formal aspects of the *TB-LMTO* and the *Screened KKR method* are reviewed in terms of multiple scattering theory (Scattered Wave Method) as based on a general reference medium. In terms of the corresponding Green's functions a comparison is made between these two approaches listing similarities and differences, advantages and disadvantages.

(submitted to Int. J. of Quantum Chemistry)  
Manuscripts available from: pw@eecs1.tuwien.ac.at

\*)Dedicated to the memory of Jean Louis Calais

# Ab-initio theory of surface segregation: self-consistent determination of the concentration profile

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## Abstract

The parameters of the effective Ising Hamiltonian governing segregation and ordering phenomena in the surface region of an alloy are determined from first principles. Employing the force theorem, the total energy of semi-infinite disordered alloys is mapped onto an Ising Hamiltonian. The band term is treated within the Generalized Perturbation Method, and, in addition, the contributions from core states, the double-counting and the Madelung terms are included. The concentration profile is determined by using Monte Carlo simulations. The electronic structure and the Ising Hamiltonian parameters are then recalculated for the new profile, and the whole procedure is repeated until self-consistency between the electronic and atomic structure of the alloy surface is achieved. As an illustration, the results for an fcc (001) surface of the Cu-Ni alloys, as calculated within the all-electron fully relativistic TB-LMTO-CPA method, are discussed.

(submitted to Phys. Rev. B)

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# Magnetic Anisotropy in Fe/Cu(001) over- and interlayers: I. The High-Moment Ferromagnetic Phase

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## Abstract

An extensive study of the magnetic anisotropy energies (MAE) of the high-moment ferromagnetic phase of fcc Fe/Cu(001) over- and interlayers is presented in terms of the fully relativistic spin-polarized Screened Korringa-Kohn-Rostoker method. Independent of the film thickness for free surfaces the orientation of the magnetization is found to be in-plane, while for capped films a perpendicular magnetization is predicted up to a switching thickness of 5 Fe monolayers. Based on an analysis of layer-resolved anisotropy energies it is shown that the main contribution to the MAE arises from the Fe layer at the Fe/Cu interfaces. Particular features of the MAE's with respect to the number of cap layers as well as to the film thickness can be viewed in terms of an interfacial hybridization between Fe and Cu. By using the coherent-potential approximation the interdiffusion between the substrate and the magnetic film is shown to reduce the MAE dramatically.

(submitted to Phys. Rev. B)

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# The Massively Parallel $O[N]$ LSMS METHOD: Alloy Energies and Non-collinear Magnetism

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## Abstract

We present an overview of the locally self-consistent multiple scattering (LSMS) method. The method is based on real space multiple scattering theory, is naturally highly parallel, and has been implemented on Intel Paragon parallel platforms within the Center for Computational Sciences at Oak Ridge National Laboratory.  $O(N)$ -scaling is demonstrated for unit cells as large as 1000-atoms. We discuss in detail how the real space convergence properties of the method can be controlled by taking advantage of the stationary properties of a finite temperature *Harris-Foulkes* free energy functional. We show how the LSMS method can be combined with the recently developed spin-dynamics to treat non-collinear magnetic states of materials. We show some preliminary results for the ground state magnetic structure of FCC  $\text{Fe}_{0.65}\text{Ni}_{0.35}$  alloys that indicate the possible existence of non-collinear arrangements of magnetic moments in this system.

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# Density dependence of the electronic supershells in the homogeneous jellium model

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## Abstract

We present the results of self-consistent calculations of the electronic shell and supershell structure for clusters having up to 6000 valence electrons. The ionic background is described in terms of a homogeneous jellium. The calculations were performed for a series of different electron densities, resembling Cs, Rb, K, Na, Li, Au, Cu, Tl, In, Ga, and Al, respectively. By analyzing the occupation of the energy levels at the Fermi energy as a function of cluster size, we show how the shell and supershell structure for a given density arises from the specific arrangement of energy levels. We investigate the electronic shells and supershells obtained for different electron densities. Using a scaling argument, we find a surprisingly simple dependence of the position of the super-nodes on the electron density.

(submitted to Phys. Rev. B)  
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# Superlattices and interfaces X/Cu (X=Fe, Co, Ni): Calculation and interpretation of magnetic properties

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## Abstract

We study the different magnetic behaviours of Fe, Co and Ni with respect to bulk properties when forming superlattices with Cu and when one monolayer is deposited on Cu(001). We look at the contribution to the magnetic moment coming from the different orbital symmetries which is nowadays experimentally measured. Based on a qualitative analysis of paramagnetic model densities of states we show that the distinct magnetic behaviours are due essentially to band filling.

(submitted to Phys. Rev. B)  
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# Calculation of the magnetoresistance in RhFe

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## Abstract

We have calculated the diffusive conductivity and the ballistic conductance of three different magnetic configurations of *RhFe* within the semiclassical theory of conduction. Both magnitudes lead to a large magnetoresistance in agreement with experimental results although they correspond to different transport regimes.

(accepted by Phys. Rev. B)

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# TRANSPORT PROPERTIES OF Co-Ni SUPERLATTICES

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## Abstract

In this paper we calculate the ballistic conductance  $G$  and the diffusive conductivity  $\sigma$  for Co-Ni superlattices grown in the (111) direction, with the intention of investigating the effect of the superlattice band structure on the electric transport properties. The calculation was carried out in the framework of the semiclassical approximation (Boltzmann's equation). A Hubbard tight-binding Hamiltonian, solved in the Hartree-Fock approximation, and parametrized to fit bulk equilibrium values, was used to obtain the band structure. The presence of interfaces reduces the in plane and, more strongly, the perpendicular to the plane electric conduction, even when impurity scattering is disregarded. The results for  $G$  and  $\sigma$  show qualitative differences and thus, in the interpretation of the experiments, it is important to ascertain the precise nature of the transport regime.

(submitted to Phys. Rev. B)

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# Magnetic dimers of transition metal atoms on the Ag(001) surface

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## Abstract

The magnetic properties of transition metal dimers on Ag(001) are calculated in local spin density approximation by means of a KKR Green's function technique. It is shown, that many transition metals, which are nonmagnetic in their bulk form, are magnetic as dimers on the Ag(001) surface. The surface-dimer interaction is studied by comparing the magnetic moments of supported and free dimers. The increased *sp-d* hybridisation with the substrate strongly decreases the magnetic moments of *4d* and *5d* dimers in comparison with the *3d* ones. However, also for these series magnetic dimers with large moments exist.

(submitted to Phys. Rev. B)

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## Acknowledgement

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# Compton-scattering study of the electronic properties of the transition-metal alloys FeAl, CoAl and NiAl

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## Abstract

Directional Compton profiles of the transition-metal alloys FeAl, CoAl and NiAl have been measured. Both conventional technique (resolution 0.55 a.u. of momentum), based on a 59.3 keV x-ray source with a solid-state detector and a high-resolution spectrometer (0.15 a.u. of momentum) with 50 keV x-rays from a synchrotron source have been used. The results are interpreted using a theory based on a full potential linearized augmented plane wave method. The agreement between the experimental and the theoretical momentum density anisotropy is very good. It is shown that the anisotropies at low momenta are heavily influenced by the particular shape of the Fermi surface.

(Phys. Rev. B **53**, 7714 (1996))

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# Role of Covalent Tip–Surface Interactions in Non–contact AFM on Reactive Surfaces

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## Abstract

Total–Energy pseudopotential calculations are used to study the imaging process in non–contact Atomic Force Microscopy on Si(111) surfaces. The atomic resolution seen in some parts of the experimental images is attributed to the onset of covalent bonding between a localised dangling bond on the atom at the apex of the tip and the dangling bonds on the adatoms in the surface. This interaction dominates the force gradients, which drive the frequency changes used to create the experimental images, and provides a mechanism for atomic resolution imaging on reactive surfaces.

R. P. acknowledges the financial support of the Human Capital and Mobility Programme of the European Union under contract ERBCHRXCT930369 (HCM  $\psi_k$ -Network on Ab initio (from electronic structure) calculation of complex processes in materials).  
(submitted to Phys. Rev. Lett.)

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# Effect of Interface Magnetic Moments and Quantum Well States on Magnetization Induced Second Harmonic Generation

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## Abstract

We develop a model for magnetization induced second harmonic generation (MSHG) experiments on Co/Cu(001) and Cu/Co(001) overlayers by expanding the non-linear optical susceptibility to lowest order in the magnetization, and taking the latter to be given by the interfacial moments from *ab-initio* electronic structure calculations. The model accounts well for the relative MSHG signal from Co/Cu(001), but contrary to experiment predicts a nearly constant signal for Cu/Co(001). We discuss the possibility of quantum well states accounting for the failure in the latter case.

(submitted to Phys. Rev. B)

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# Magnetocrystalline anisotropy of $\text{YCo}_5$ and related $\text{RECo}_5$ compounds

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## Abstract

The magnetocrystalline anisotropy energy of  $\text{YCo}_5$  has been calculated from first principles using the local-spin-density approximation. The easy magnetization axis is predicted correctly and the anisotropy energy is only 20% smaller than the experimental value if a recently proposed orbital polarization correction is included; otherwise it is about a factor of seven too small. Our analysis indicates that magnetic materials with substantially larger anisotropy energies than the best available nowadays should be possible. A large orbital moment is found to contribute to the magnetization bringing the calculated moment,  $8.0 \mu_{\text{B}}$  per  $\text{YCo}_5$  unit cell, into good agreement with the experimental value of  $8.3 \mu_{\text{B}}$ . A large anisotropy in the magnetization is calculated which is nearly completely due to an anisotropic orbital moment associated with the Co atoms. The magnetocrystalline anisotropy energy is shown to be strongly correlated with the anisotropy in the total orbital moment. There is a large reduction in the hyperfine fields compared to the value in bulk hcp Co, not only due to large orbital contributions, but also to different values of the valence contact term.

The contribution of the rare-earth (RE) ions to the anisotropy energy of the related  $\text{RECo}_5$  compounds may be understood in terms of the crystal field and exchange interactions felt by the localized RE(4f) electrons. The RE(4f)-Co exchange interactions and the Hartree contribution to the crystal field have been calculated under the assumption that these interactions may be treated as small perturbations. The electric field gradient  $V_{zz}$  and the  $A_2^0$  crystal field parameter at the RE site are a factor of two and three larger than the experimental values, respectively. The order of magnitude of the calculated exchange field agrees with the values derived from experiment.

(accepted for publication in Physical Review B)  
Manuscript available from [kelly@natlab.research.philips.com](mailto:kelly@natlab.research.philips.com)

# Band Structure Calculations of Ferromagnetic Chromium Tellurides CrSiTe<sub>3</sub> and CrGeTe<sub>3</sub>

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## Abstract

Band structure calculations using the spin-polarized ASW method were performed on the title compounds. Non-metallic behavior is attributed to spin-polarization-induced opening of a gap at the Fermi level. Curie temperatures were calculated, on the basis of an Ising model. The results are found in reasonable agreement with the real evolution of silicon and germanium derivatives.

(in press in Journal of Phys. Chemistry, **100**, 1996)  
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# *Ab initio* calculations of the cohesive, elastic and dynamical properties of $\text{CoSi}_2$ by pseudopotential and all-electron techniques

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## Abstract

*Ab initio* calculations of cohesive properties, elastic constants and phonon dispersions for  $\text{CoSi}_2$  were performed by means of the Vienna *ab initio* molecular dynamics package (VAMP) which makes use of ultrasoft pseudopotentials. In addition, the all-electron full-potential linearized augmented plane wave (FLAPW) method was used for the calculation of equilibrium properties as well as elastic constants derived from second derivatives of total energies. For both methods, total energies, their derivatives and related quantities are fully converged with respect to basis sizes and number of  $\vec{k}$  points. Our results for  $C_{44}$  prove that atomic positions in the strained crystal have to be fully relaxed in order to get quantitative useful results. The results of both methods obtained within the same type of local density approximation (LDA) are in very good agreement between each other. Because elastic constants are very sensitive quantities for an *ab initio* method in general, the reproduction of high quality all-electron data by VAMP demonstrates the power of suitably constructed pseudopotentials even for systems containing transition elements. VAMP was also applied to calculate elastic constants in two other ways, namely directly from the stress-strain relations (which yielded the same results as obtained from total energy derivatives) and from acoustic branches of the phonon dispersion. In this case, however, we only succeeded to get a useful result for  $C_{44}$  whereas for the remaining two elastic constants prohibitively large supercells would be needed. Finally, VAMP calculations were performed within the framework of the generalized gradient approximation (GGA) to density functional theory. By that, data were derived which are in very good agreement with experimental values.

(Phys. Rev. B, submitted)

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# Scanning Tunneling Spectroscopy of One-dimensional Surface States on a Metal Surface

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## Abstract

Scanning tunneling spectroscopy permits real-space observation of one-dimensional electronic states on a Fe(100) surface alloyed with Si. These states are localized along chains of Fe-atoms in domain boundaries of the Fe(100) c(2 × 2)Si surface alloy, as confirmed by first-principles spin-polarized calculations. The calculated charge densities illustrate the d-like orbital character of the one-dimensional state and show its relationship to a two-dimensional state existing on the pure Fe(100) surface.

(Phys. Rev. Lett., submitted)

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# Efficiency of *ab-initio* total energy calculations for metals and semiconductors using a plane-wave basis set

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## Abstract

We present a detailed description and comparison of algorithms for performing *ab-initio* quantum-mechanical calculations using pseudopotentials and a plane-wave basis set. We will discuss: (a) Partial occupancies within the framework of the linear tetrahedron method and the finite-temperature density-functional theory, (b) iterative methods for the diagonalization of the Kohn-Sham Hamiltonian and a discussion of an efficient iterative method based on the ideas of Pulay's residual minimization, which is close to an order  $N_{\text{atoms}}^2$  scaling even for relatively large systems, (c) efficient Broyden-like and Pulay-like mixing methods for the charge density including a new special 'preconditioning' optimized for a plane-wave basis set, (d) conjugate gradient methods for minimizing the electronic free energy with respect to all degrees of freedom simultaneously. We have implemented these algorithms within a powerful package called VAMP (Vienna *ab-initio* molecular-dynamics package). The program and the techniques have been used successfully for a large number of different systems (liquid and amorphous semiconductors, liquid simple and transition metals, metallic and semi-conducting surfaces, phonons in simple metals, transition metals and semiconductors) and turned out to be very reliable.

(to appear in Computational Materials Science)  
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# Atomic and electronic structure of diamond (111) surfaces: II. $(2 \times 1)$ and $(\sqrt{3} \times \sqrt{3})$ reconstructions of the clean and hydrogen-covered three-dangling-bond surfaces

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## Abstract

We present *ab-initio* local-density functional calculations of the atomic reconstruction of clean and hydrogen-covered three-dangling-bond (3db) diamond (111) surfaces, extending our earlier work on the one-dangling-bond surface. 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. For the bulk-terminated surfaces we predict a difference of 1.90 eV/atom in the cleavage energies of the 1db and 3db surfaces (also referred to as shuffle- and glide-plane cleavage), i.e. considerably less than expected from a simple bond-scission argument. This difference is further reduced by reconstruction. We find that the clean C(111)-3db surface reconstructs in a  $(2 \times 1)$  geometry with symmetric, unbuckled  $\pi$ -bonded chains (Seiwatz-chains), but a pronounced buckling in some of the deeper layers. However, a  $(\sqrt{3} \times \sqrt{3})$ -reconstruction with the surface atoms forming slightly buckled trimers is energetically less favourable by only 0.12 eV/atom. Hydrogenation of the surface stabilizes the  $(2 \times 1)$  geometry of the surface relative to the  $(\sqrt{3} \times \sqrt{3})$  geometry. Deposition of a monolayer of hydrogen does not change the single-chain topology of the surface. A hydrogen-coverage of 2 H-atoms per surface C-atom leads to the formation of parallel rows of  $C_2H_4$  units arranged again in a  $(2 \times 1)$  geometry. A coverage of 3 H-atoms per C-atom leads to a complete de-reconstruction and stabilizes a  $(1 \times 1)$  C(111)-3db surface (which is identical to a C(111)-1db  $(1 \times 1)$  surface covered with  $CH_3$  groups). Our calculations show that at larger values of the hydrogen chemical potential, the strongly hydrogenated 3db surfaces are stabilized over the 1db surface.

(submitted to Surf. Science)

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# Adatom self-diffusion processes on (001) copper surface by molecular dynamics

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## Abstract

Using molecular dynamics and an n-body potential adapted to copper we have studied the self-diffusion of Cu adatoms on Cu (001) surface. The simulations covered the temperature range between 700K and 1100K. Besides the simple hopping and the exchange mechanism, the detailed trajectory analysis revealed multiple hopping events and complicated multi-particle exchange processes, involving several atoms that do not necessarily belong to the same nearest-neighbor row. These processes exhibit Arrhenius behavior from which we derived the migration energies associated with each process. It is found that the hopping mechanism requires an energy of 0.43eV, in very good agreement with available experimental data, while the energy associated with the exchange mechanism is 0.70eV. These results are in qualitative agreement with recent ab-initio calculations. In addition, we found that all mechanisms, even the most complicated, require about the same migration energy with the simple exchange and that for temperatures above 900K they contribute almost equally to the total diffusion. Furthermore, the activation barriers for the hopping and the exchange mechanism deduced from energy minimization, at T=0K, compare well with the simulation values.

(in Surf.Sci. 347, 376 (1996))

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# Atomic Modelling of Nb, V, Cr, and Mn Substitutions in $\gamma$ -TiAl

## 2: Electronic Structure and Site Preference

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### Abstract

The effect of Nb, V, Cr, and Mn on the lattice parameters of  $\gamma$ -TiAl and the site preference of these transition metals were studied based on first-principles supercell calculations of the electronic structure and total energy of ordered  $\text{Ti}_{n-1}\text{XAl}_n$  and  $\text{Ti}_n\text{XAl}_{n-1}$  compounds with  $\text{X} = \text{Nb, V, Cr, and Mn}$ . For the calculation of optimized volumes by total energy minimization 4-, 8- and 32-atom cells were taken into account. Trends of  $c/a$  changes in connection with the analysis of the electronic structure are derived from 4-atom supercell results in continuation of a previously published part 1 of our investigations. We find that Mn has the strongest preference for Al sites because of strong stabilizing electronic structure effects. The substantial decreased value of the  $c/a$  ratio found for the case of Mn substituting for Al is related to a bcc-like lokal arrangement of Ti around the Mn atom. This geometrical situation is accompanied by the formation of a deep pseudogap in the density of states. The Fermi energy falls precisely into this pseudogap which distinctly separates Ti-Mn bonding and antibonding states. The site preference trend for the other substitutional compounds containing  $\text{X} = \text{Nb, V, Cr}$  are also discussed in combination with their corresponding density of states.

Intermetallics 4, 201 (1996)  
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## Presenting Other Initiatives

### News from the Centre Européen de Calcul Atomique et Moléculaire

The *Centre Européen de Calcul Atomique et Moléculaire* (CECAM) is a research center for the study and application of computational methods in physics and chemistry. The scientific scope of CECAM spans from Condensed-Matter Physics to Materials Science, Statistical Mechanics, Quantum Chemistry, Atomic and Molecular Physics, and the Physics of Biomolecules.

The Center was founded in 1969 and has played a significant role in the development of computational physics and chemistry in Europe, especially in the field of classical simulations. In 1994 CECAM moved from its original site, Orsay near Paris, to Lyon, France, where it is now hosted by the *Ecole Normale Supérieure de Lyon* which provides a very convenient scientific environment. Little later, the directorship was taken over by Stefano Baroni who will stay in charge until 1998. The present director is committed to strengthen the role of CECAM in some of those scientific areas not so well represented in its past activities, while keeping and enhancing the level of excellence already established in the field of classical simulations.

CECAM is based on a collaboration among several European National Science Foundations. The following institutions are currently members of the Centre:

- *Centre National de la Recherche Scientifique* (CNRS), France;
- *Commissariat à l'Energie Atomique* (CEA), France;
- *Consiglio Nazionale delle Ricerche* (CNR), Italy;
- *Ecole Normale Supérieure de Lyon* (ENSL), France;
- *Fonds National de la Recherche Scientifique* (FNRS), Belgium;
- *Fonds National Suisse* (FNS), Switzerland;
- *Foundation for Research and Technology Hellas* (FORTH), Greece;
- *Istituto Nazionale di Fisica della Materia* (INFM), Italy;
- *Nederlandse Organisatie voor Wetenschappelijk Onderzoek* (NWO), The Netherlands;
- *Engineering and Physical Sciences Research Council* (EPSRC), United Kingdom.

A major commitment of the present director is to extend the participation in CECAM to Germany and to other European countries. Scientists from non-member countries who believe that their national scientific community would benefit from joining CECAM are particularly encouraged to get in touch with Stefano Baroni and to put forward suggestions on how to achieve this goal.

The main activity of CECAM is the organization of study meetings on specific topics within its scope. The preference is given to those meetings which aim either to explore new fields of research or to put in contact different scientific communities that, while having common interests, do not interact very much. The choice of the format is left to the organizers' responsibility, and it is usually rather informal with ample space left to discussion and personal interactions. Although CECAM can accommodate a larger number of participants, the usual number of attendees ranges between 15 and 30. The duration of the meetings spans from 3 days to 2 weeks. The budget allocated to each meeting varies accordingly between 40,000 and 80,000 French Francs. So far, the vast majority of the CECAM meetings has been entirely funded by CECAM itself. It is hoped that in the future CECAM could host meetings cosponsored by other organizations.

Participation in CECAM's activities is not restricted to scientists from member countries. As a matter of fact, during 1995 roughly 50% of the participants of the CECAM's study meetings as well as several of the organizers came from other countries. Proposals for CECAM's workshops are solicited for submission to the director every year by August 31. The director organizes a peer review which is then submitted together with the proposals to the Scientific Council that gathers in November and makes the final decision on next year's program.

The CECAM's scientific program for 1996 will include:

- *Development of transferable intermolecular potentials for phase equilibrium calculations*, organized by P. T. Cummings, Oak Ridge National Laboratory, USA, and A. Z. Panagiotopoulos, Cornell University, USA. 13–15 May.
- *Non-perturbative methods for solving time dependent problems of atoms and molecules in strong fields*, organized by P. Lambropoulos and D. Charalambidis, Institute of Electronic Structure and Laser, Crete, Greece. To be held in Crete, 27–29 May.
- *Pattern formation in surface reactions*, organized by L. M. Sander, University of Michigan, USA, E. Clément, Université Pierre et Marie Curie, Paris, France, and A. Blumen, Universität Freiburg, Germany. 3–6 June.
- *Theoretical predictions of alloy phase stability* organized by A. Zunger, National Renewable Energy Laboratory, Golden Colorado, USA, and A. Finel, ONERA, Chatillon, France. 10–14 June.
- *Algorithms for dynamic critical phenomena*, organized by W. Janke, Johannes Gutenberg Universität, Mainz, Germany. 20–22 June.
- *Integral equations for the pair structure of classical and quantum fluids: state of the art and recent applications* organized by M. Rovere, Università della Calabria, Italy, J. -P. Hansen, Ecole Normale Supérieure de Lyon, France, and G. Pastore, Università di Trieste, Italy. 26–29 June.
- *Ab-initio phonons*, organized by X. Gonze, Université Catholique de Louvain, Belgium, P. Giannozzi, Scuola Normale Superiore, Pisa, Italy, and H. Krakauer, College of William and Mary, Williamsburg, USA. 1–3 July.
- *Grid, multigrid and wavelet methods in structure electronic calculations*, organized by J. F. Annett, University of Bristol, UK, and J. Bernholc, North Carolina State University, USA. 4–6 July.
- Euroconference on *The microscopic approach to complexity in non-equilibrium molecular simulations*, organized by M. Mareschal, Université Libre de Bruxelles, Belgium, and B. L. Holian, Los Alamos National Laboratory, USA. 15–19 July.
- *Models and computer simulations for electrokinetic phenomena*, organized by P. Turq, Université Pierre et Marie Curie, Laboratoire d'Electrochimie, Paris, France, L. Blum, University of Puerto Rico, USA, and M. Mareschal, Université Libre de Bruxelles, Belgium, within the EU HCM network *Molecular Dynamics and Monte Carlo Methods for Quantum and Classical Systems*. 22–26 July.
- *High performance computational chemistry*, organized by A. Sgamellotti and F. Tarantelli, Università di Perugia, and M. F. Guest, Daresbury Laboratory, UK. 5–7 September.
- *Going beyond the local density approximation in physics and chemistry*, organized by C. Umrigar, Cornell Theory Center, Cornell University, Ithaca, USA, A. Savin, Laboratoire de Dynamique des Interactions Moléculaires, Université Pierre et Marie Curie, Paris, France, and U. von Barth, Department of Theoretical Physics, University of Lund, Sweden. 9–13 September.
- *The interaction of ultra-intense short pulses lasers with plasmas*, organized by M. G. Haines, Imperial College, London, UK, G. Bonnaud, CEA, Limeil-Valenton, France, and A. R. Bell, Imperial College, UK. 16–20 September.
- *Potential functions for simulation of biomolecules*, organized by M. Marchi and J. C. Smith, CEA, Saclay, France, and M. L. Klein, University of Pennsylvania, USA. 23–25 September.



- *Glassy dynamics*, organized by J.-P. Bouchaud, CEA, Saclay, France, L. Cugliandolo, CEA, Saclay, France, J. Kurchan, Ecole Normale Supérieure, Paris, France, and M. Mézard, Ecole Normale Supérieure, Paris, France. 30 September – 4 October.

Besides the organization of study meetings, CECAM hosts a small but well established local research activity. Current research fields include the simulation of photosynthetic reaction centers in biological molecules, non-adiabatic effects in chemical reactivity, large-scale electronic-structure calculations, and ab-initio molecular-dynamics simulations. During 1995 seven post-docs and graduate students have been working at CECAM under the supervision of the director and/or of external senior scientists. This number is obviously subject to fluctuations. Collaborations with external institutions willing to provide partial support to the stay of young researchers at CECAM are especially encouraged. These collaborations may also include regular visits to CECAM of senior scientists who can act as supervisors of the research carried on by the young researchers. Scientists at CECAM have access to both local and remote computer resources. The former include a cluster of six DEC Alpha stations, an IBM 58H POWER2 station, and a 16-processor CONVEX EXEMPLAR SPP-1000 parallel machine belonging to the Ecole Normale Supérieure de Lyon. Furthermore, CECAM has access to several European supercomputing centers.

One of the important aims of CECAM is to contribute to the development of emerging research fields in computational physics and chemistry, which are not yet well represented in Europe. This is pursued also by encouraging scientists well established in one of these fields to spend a sabbatical visit at CECAM. During 1995 one of such programs has been started in collaboration with D. Coker (Boston University, USA) in the field of *Nonadiabatic dynamics and chemical reactivity*. A position for a six-months sabbatical visit during 1996 is available. Interested scientists are invited to get in touch with the director.

An up-to-date summary of the CECAM's activities is available on the World-Wide Web at URL address-<http://www.cecarn.fr/>. People wishing to contact the director can do so by e-mail at the address: [baroni@cecarn.fr](mailto:baroni@cecarn.fr).

## Non-collinear magnetism: effects of symmetry and relativity

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### Abstract

We give a brief review of the theory of non-collinear order in itinerant electron systems. The theory is an example of the use of the local density-functional approximation for first-principles calculations. We emphasize the role of symmetry arguments since they facilitate the calculations and make the physics of the problem transparent. We choose as examples spiral structures like those found experimentally in fcc Fe, the canted states of  $U_3P_4$  and weak ferromagnetism in  $\alpha\text{-Fe}_2\text{O}_3$  and show that these different phenomena are explained by the theory.

## 1 Introduction

It was more than forty years ago that non-collinear magnetic structures were first discovered experimentally [1], yet this physical phenomenon was investigated theoretically almost entirely in the framework of model Hamiltonians, assuming localized atomic moments [1], in contrast to collinear magnets which were intensively studied using first-principles calculational schemes provided by the density functional theory [2, 3]. This is perhaps due to the fact that non-collinear magnetic order seemed rather exotic and rare. But it attracted renewed interest in the late seventies and beginning of the eighties when it became clear that Stoner theory, which explains ground-state properties quite well, fails to describe the temperature behaviour of itinerant magnets. The reason for this failure was found in the neglect of transverse fluctuations of the magnetization density that, if viewed as originating from well-formed atomic moments, is equivalent to neglecting fluctuations in the directions of atomic moments (see e.g. [4]).

Detailed investigations of particular non-collinear magnetic configurations were started by Heine and his group using the cluster recursion method applied to a simplified tight-binding Hamiltonian [5]. The line of this work was continued with the use of the KKR method for a periodic solid (see e.g. [6]). A thorough discussion of density functional theory for a non-collinear magnet was subsequently given in [7] and applied to investigate the ground-state electronic and magnetic structure of  $Mn_3Sn$ . It was the experimental discovery of a spiral magnetic structure in fcc Fe [8] that made Fe an interesting object for theoretical studies [9, 10]. The last years showed a boom in investigations of non-collinear magnetism. Thus, for instance, successful studies of disordered systems [11, 12, 13] as well as multilayers [14, 15] were reported and a noteworthy and interesting step was made in describing the spin dynamics in itinerant electron systems [16]. In spite of its rather short history the theory of non-collinear magnetism involves quite different methods and is applied to a multitude of different physical problems. In this brief review we

are not trying to discuss all aspects of the presently used first-principles studies of non-collinear magnets, but rather select aspects which possess interesting symmetry properties. In particular, we will expose the role of spin-orbit coupling. This relativistic interaction sometimes acts in a destructive, sometimes in a constructive, way in the formation of particular non-collinear magnetic structures.

## 2 Kohn-Sham Hamiltonian of a non-collinear magnet

The derivation of the Kohn-Sham Hamiltonian for non-collinear magnets follows the standard procedure of density functional theory. In this case the total energy is considered as a functional of the two-dimensional density matrix and all single-particle wave functions are consequently treated as two-component spinor functions [7]. After variation of the functional with respect to the components of the spinor function one obtains equations that describe a magnetization continuously varying in space. For practical calculations it is common to use the atomic sphere approximation for the magnetization direction, i.e. the direction of the magnetization is supposed to be constant within the atomic sphere of every atom and different for different atoms. The scalar-relativistic Hamiltonian of a non-collinear magnet then takes the form

$$\hat{\mathbf{H}}_{sc}(\mathbf{a}_\nu, \mathbf{e}_\nu) = \sum_\nu \mathbf{U}^+(\theta_\nu, \phi_\nu) \begin{pmatrix} H_{sc}^{\nu\uparrow}(\mathbf{r}_\nu) & 0 \\ 0 & H_{sc}^{\nu\downarrow}(\mathbf{r}_\nu) \end{pmatrix} \mathbf{U}(\theta_\nu, \phi_\nu) \quad . \quad (1)$$

Here  $\mathbf{a}_\nu$  are atomic positions and  $\mathbf{e}_\nu$  directions of atomic moments,  $\mathbf{U}(\theta_\nu, \phi_\nu)$  is the standard spin- $\frac{1}{2}$ -rotation matrix, which describes the transformation between a global and a local coordinate system of the  $\nu$ th atom, whose spin orientation is given by the polar angles  $\theta_\nu$  and  $\phi_\nu$  with respect to the z-axis of the global system. The quantities  $H_{sc}^{\nu\uparrow}(\mathbf{r}_\nu)$  and  $H_{sc}^{\nu\downarrow}(\mathbf{r}_\nu)$  are the standard atomic scalar-relativistic Hamiltonians (spin up, spin down) [17] in the local frame of reference for the atom at site  $\nu$ . They contain the mass-velocity, the Darwin term and the effective one-particle potential which, as usual, is given by functional derivatives of the total energy and is spin-diagonal in the local frame of this atom.

Note that the scalar-relativistic Hamiltonian possesses the same symmetry properties as the non-relativistic Hamiltonian which is obtained from the former by neglecting the mass-velocity and Darwin terms. Therefore the symmetry aspects discussed in this paper will be equally valid for both cases. Our calculations were carried out with the scalar-relativistic Hamiltonian.

A substantial part of the discussion will be devoted to the role of spin-orbit coupling which we will write in the form

$$\hat{\mathbf{H}}_{so} = \sum_\nu \mathbf{U}^+(\theta_\nu, \phi_\nu) \left\{ \sum_\alpha M_\alpha \sigma_\alpha \hat{l}_\alpha \right\} \mathbf{U}(\theta_\nu, \phi_\nu). \quad (2)$$

Here  $\sigma_\alpha$  and  $\hat{l}_\alpha$  are the Cartesian components of the Pauli spin matrices and the angular momentum, respectively, in the local system and the coefficients  $M$  can be found in Ref. [18].

The purpose of our work is the first-principles determination of the magnetic structure of a crystal. The basic steps to achieve this can be summarized as follows [7]: in each iteration step

the eigenstates  $\begin{pmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{pmatrix}_i$  of the Hamiltonian  $\hat{\mathbf{H}}_{sc}$  in the scalar-relativistic or  $\hat{\mathbf{H}}_{sc} + \hat{\mathbf{H}}_{so}$  in the relativistic case are calculated which enables us to determine the two-dimensional density matrix of the system:

$$\rho(\mathbf{r}) = \sum_{i \text{ occ}} \begin{pmatrix} \psi_1(\mathbf{r})^* \psi_1(\mathbf{r}) & \psi_1(\mathbf{r})^* \psi_2(\mathbf{r}) \\ \psi_2(\mathbf{r})^* \psi_1(\mathbf{r}) & \psi_2(\mathbf{r})^* \psi_2(\mathbf{r}) \end{pmatrix}_i \quad (3)$$

where the sum runs over all occupied states. The density matrix contains information on the charge density, the directions of the atomic magnetic moments and the magnetization, all of which are necessary to redetermine the Hamiltonian for the next iteration step. The iterations are repeated until full self-consistency is achieved. The new degrees of freedom connected with the variation of the direction of the magnetic moments make the problem numerically more involved than in the case of a collinear magnetic state.

### 3 Generalization of the symmetry basis

Traditionally the symmetry properties of non-relativistic Hamiltonians are described in terms of ordinary irreducible representations of the relevant space group whereas for the relativistic problem the so-called double-valued irreducible representations are used. However, this difference in the type of representation merely reflects the difference in the choice of the functions subjected to the transformation. In the relativistic case the transformed function is always a spinor function whereas it is a scalar wave function in the non-relativistic case for which, correspondingly, only the transformation properties in real space need be considered.

It is the spinor form of the wave function that is of prime importance for the case of non-collinear magnetism. Hence, as in the relativistic case, one must use the double-valued irreducible representation. Still there is a subtle difference in the symmetry properties of the problem depending on whether or not the spin-orbit coupling is retained in the Hamiltonian. To describe this properly one introduces a generalized set of operators which allows an independent transformation of the spin and space variables [19]. For the group of such operators we will use the term spin-space group (SSG).

We define the action of an operator of the SSG on a two-component spinor function as follows

$$\{\alpha_S|\alpha_R|\mathbf{t}\} \psi(\mathbf{r}) = U(\alpha_S) \psi(\{\alpha_R|\mathbf{t}\}^{-1}\mathbf{r}) \quad (4)$$

where  $\psi$  is a two-component spinor function,  $U$  is the spin- $\frac{1}{2}$ -rotation matrix,  $\alpha_S$  and  $\alpha_R$  are, respectively, spin and space rotations, and  $\mathbf{t}$  is a space translation. Operators of the usual space group are those with  $\alpha_S = \alpha_R$ .

One easily proves that a transformation of the scalar-relativistic Hamiltonian (i.e. not including spin-orbit coupling) of a non-collinear magnet with the operations (4) leaves the form of the Hamiltonian invariant, i.e.

$$\hat{\mathbf{H}}_{sc}(\mathbf{a}'_\nu, \mathbf{e}'_\nu) = \{\alpha_S|\alpha_R|\mathbf{t}\} \hat{\mathbf{H}}_{sc}(\mathbf{a}_\nu, \mathbf{e}_\nu) \{\alpha_S|\alpha_R|\mathbf{t}\}^{-1} \quad (5)$$

where  $\mathbf{a}_\nu$  are atomic positions and  $\mathbf{e}_\nu$  directions of atomic moments corresponding to the untransformed Hamiltonian. From (5) it follows that two magnetic crystals with atomic positions connected by the relation  $\mathbf{a}'_\nu = \alpha_R \mathbf{a}_\nu + \mathbf{t}$ , and directions of magnetic moment connected by  $\mathbf{e}'_\nu = \alpha_S \mathbf{e}_\nu$ , are equivalent in the scalar-relativistic case.

However, a transformation of the spin-orbit coupling term with an SSG operator does not reproduce the form of this term. Only when  $\alpha_S = \alpha_R$  do we restore the form-invariance of the Hamiltonian and find equivalent magnetic crystals:

$$\{\alpha_R|\alpha_R|\mathbf{t}\} \hat{\mathbf{H}}_{so}(\mathbf{a}_\nu, \mathbf{e}_\nu) \{\alpha_R|\alpha_R|\mathbf{t}\}^{-1} = \hat{\mathbf{H}}_{so}(\mathbf{a}'_\nu, \mathbf{e}'_\nu) \quad (6)$$

In many cases we are interested in the symmetry properties of one particular magnetic configuration and not in establishing the equivalence of different magnetic configurations. In this case the atomic positions and corresponding atomic moments must be the same before and after the transformation and the equations (5,6) reduce to commuting Hamiltonian and symmetry operators.

In what follows we will show how symmetry arguments help us to make calculations and facilitate to analyze the calculational results for a number of different physical problems.

### 4 Incommensurate spiral structure

A spiral magnetic structure is defined by

$$\mathbf{m}_n = m (\cos(\mathbf{q} \cdot \mathbf{R}_n) \sin \vartheta, \sin(\mathbf{q} \cdot \mathbf{R}_n) \sin \vartheta, \cos \vartheta) \quad (7)$$

where  $\mathbf{m}_n$  is the magnetic moment of the  $n$ -th atom and  $m$ ,  $(\mathbf{q} \cdot \mathbf{R}_n)$ ,  $\vartheta$  are polar coordinates.

An apparent difficulty for first-principles calculation of a spiral structure is the loss of periodicity with respect to lattice translations non-orthogonal to  $\mathbf{q}$ . One should notice, however, that in formula (7) all atoms of the spiral structure are equivalent, in particular, because of the equal

length of all atomic moments. But atoms can be equivalent only if they are connected by a symmetry transformation. A solution of the problem is suggested by using the operators of the SSG.

Indeed, transformations combining a lattice translation  $\mathbf{R}_n$  and a spin rotation about the z axis by an angle  $\mathbf{q}\mathbf{R}_n$  leave the spiral structure invariant. The corresponding operators  $\{\mathbf{q}\mathbf{R}_n|\varepsilon|\mathbf{R}_n\}$  commute with the Hamiltonian of the spiral structure and therefore supply a symmetry transformation of the Hamiltonian. Here  $\varepsilon$  denotes the identity operation. These generalized translations form an Abelian group isomorphic to the group of ordinary space translations by vectors  $\mathbf{R}_n$ . Therefore the irreducible representations of both groups coincide and for the eigenfunctions of the Hamiltonian (1) there exists a generalized Bloch theorem [20]

$$\{\mathbf{q}\mathbf{R}_n|\varepsilon|\mathbf{R}_n\}\psi_{\mathbf{k}}(\mathbf{r}) = \exp(-i\mathbf{k}\mathbf{R}_n)\psi_{\mathbf{k}}(\mathbf{r}) \quad (8)$$

where the vectors  $\mathbf{k}$  lie in the first Brillouin zone which is defined in the usual way by the vectors  $\mathbf{q}\mathbf{R}_n$ . These properties permit to restrict our considerations of real space to a chemical unit cell, not a supercell.

Generalizations of modern methods employing density functional theory to the case of spiral structures were done in Refs. [21] (for KKR, APW and tight binding methods), [9] (for the LMTO method), [10] (for the ASW method). This approach was successfully applied to the description of the ground state of fcc-Fe [9, 10] which was experimentally observed to have a spiral magnetic structure [8].

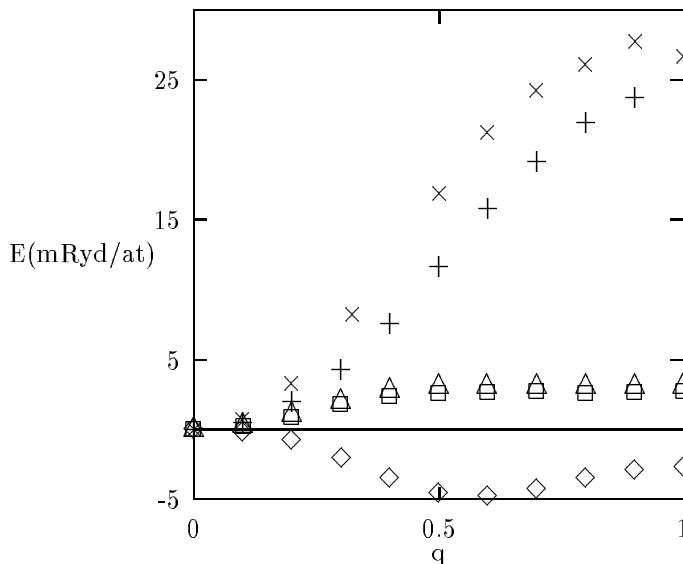


Figure 1: The total energy as a function of  $q$  for the (001) direction.  $\diamond$  - fcc-Fe;  $+$  - bcc-Fe;  $\square$  - fcc-Co;  $\times$  - hcp-Co;  $\triangle$  - Ni.

In Fig. 1 we show the results of calculations for the  $q$ -dependence of the total energy for a number of transition metals [22]. In full agreement with experiment for all metals, excluding the case of fcc-Fe, the ground state was found to be ferromagnetic which is the case of  $q=0$ . In fcc-Fe the minimum of the total energy occurs at a finite value of  $q$ , i.e. the ground state is spiral.

We complete this section with a discussion of the role of spin-orbit coupling in a spiral structure. The symmetry analysis of the previous section shows that spin-orbit coupling does not allow a separate transformation of the spin and space variables. This means the generalized translations do not apply here and we must conclude that spin-orbit coupling is destructive for the spiral structure. Indeed, experimental evidence seems to be in favour of our point of view since spiral structures are not observed in cases where the spin-orbit coupling is strong in the valence states. In particular, no spiral structures are observed in the U compounds where the U 5f electrons are itinerant and where the spin-orbit coupling is of the same order of magnitude as the exchange splitting. In contrast to this is the strong spin-orbit coupling for the core states which does not

lead to an increase of the magnetic anisotropy and therefore seems not to be an obstacle for the use of the generalized symmetry. Thus, in our opinion, the observation of spiral structures in 4f elements [1] is an argument in favour of treating the 4f states as core states.

## 5 Non-collinear magnetic structures in $U_3P_4$

Although no spiral structure was observed in U compounds there were many very different non-collinear magnetic configurations reported. To keep the length of this review acceptable we restrict the discussion to the first-principles study [23] of one interesting case namely to that of  $U_3P_4$  [24]. The magnetic moments of the individual atoms in  $U_3P_4$  do not compensate but rather possess a ferromagnetic component along the (111)-axis and the angles between the magnetic moments and the (111) axis seem to assume some accidental value. When calculations were started aligning all magnetic moments along the easy (111) axis then the scalar-relativistic and the relativistic Hamiltonians lead to drastically different results. Free to rotate, the magnetic moments deviate from the initial parallel directions in the relativistic case but stay parallel in the scalar-relativistic case. To appreciate the difference between these two cases we formulate the following nearly self-evident statement: “*The symmetry of the initial Kohn-Sham Hamiltonian must be preserved during calculations*”. This means on the one hand that if the combined symmetry of the crystal and magnetic structure is so high that a deviation of magnetic moments from the initial directions leads to perturbing the invariance of the Hamiltonian with respect to at least one symmetry operator this deviation cannot take place. On the other hand, if a deviation of the magnetic moments from the initial directions is allowed by all symmetry operations present, then there are no symmetry reasons for keeping the initial magnetic configuration and the magnetic moments will start to rotate tending to assume the state of lowest total energy. This simulated annealing of magnetic moments will continue until the “accidental” - from a symmetry point of view - ground state magnetic structure will be found by the system.

These general statements will help us to explain the behaviour of magnetic moments in  $U_3P_4$ . We start with the scalar-relativistic case. As was shown in Sect. 3 the symmetry basis of a scalar-relativistic problem is formed by the spin-space group, i.e. separate transformations of the spin and space variables are allowed. We can formulate the result in a very general way: starting the scalar-relativistic calculation with a collinear configuration we will never obtain a deviation of magnetic moments from the initial direction. Indeed, independent of the crystal structure any spin rotation by an arbitrary angle  $\phi$  about the direction of the magnetic moments  $\{C_\phi|\varepsilon|0\}$  is a symmetry operation. This group of symmetry operations gives the symmetry basis for treating the spin projection of an electron state as a good quantum number [19]. Deviations of any magnetic moment from this direction would destroy the symmetry with respect to operations  $\{C_\phi|\varepsilon|0\}$  and are therefore forbidden.

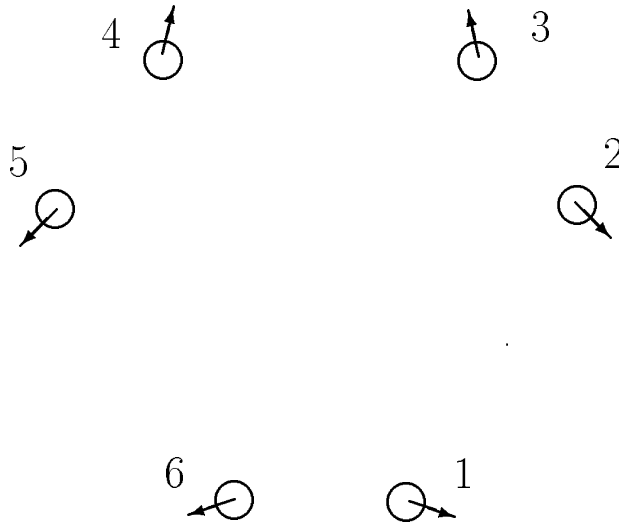


FIG. 2. Projection of the atomic positions and magnetic moments of the U atoms in  $U_3P_4$  onto the (111) plane.

The situation changes drastically in the presence of SOC because of the reduction of the symmetry basis from the SSG to the usual space groups which transforms spin and space variables in an identical way i.e.  $\alpha_S = \alpha_R$  in Sec.3. This means that the question of stability of a magnetic structure cannot be answered without analysis of the particular crystal structure. Therefore we note that  $U_3P_4$  has a bcc lattice with a basis formed by two formula units, i.e. the unit cell consists of six U and eight P atoms. The crystal structure is rather complicated and need not be discussed here in detail. Instead, to illustrate the important symmetry properties it is sufficient to consider the simple picture of Fig. 2 where the projections onto the (111) plane of the positions of the six U atoms are shown. Let us assume that initially all magnetic moments are parallel to the (111) axis which is perpendicular to the plane of the paper. Then the following operations leave the magnetic and crystal structures invariant: the rotations by  $120^\circ$  and  $240^\circ$  about the (111) axis and the reflections in the planes containing the (111) axis accompanied by time reversal. Of importance is the observation that none of these operations leaves the position of any particular atom unchanged. Because of this, symmetry imposes no restrictions on the direction of the magnetic moment of a particular atom but only on the orientation of the atomic moments relative to each other and to the crystal lattice. The deviation of the moments from the (111) axis resulting in a non-collinear magnetic configuration does not change the symmetry of the crystal. Therefore, the ferromagnetic ( $\theta=0$ ) structure, from a point of view of symmetry, is not isolated from structures possessing a non-zero  $\theta$ . In Fig. 2 we show the projections of the magnetic moments on the (111) plane which are obtained in the self-consistent calculation; these calculated deviations from the (111) axis evidently do not destroy the symmetry of the atomic configuration.

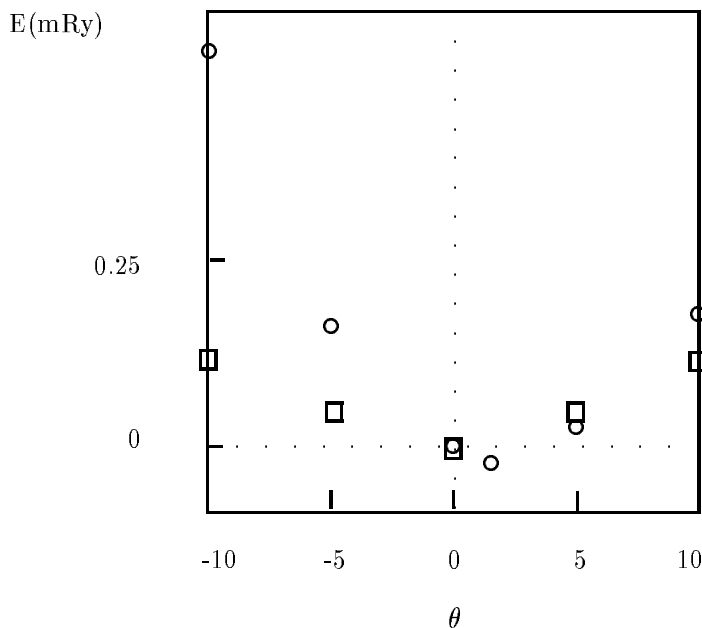


FIG. 3 Total energy of  $U_3P_4$  as a function of angle  $\theta$ . Circles show the points calculated with and squares without SOC.

More understanding of the system's behaviour can be gained with the help of Fig. 3 which shows the result for total energies when the directions of the magnetic moments are constrained to some values of angle  $\theta$  near equilibrium ( $\theta$  is the deviation of magnetic moments from the (111) direction). (During the variation of the magnetic structure we keep each moment in the plane containing the ground state direction of this moment and the (111) axis.) Fig. 3 shows that scalar-relativistic calculations give a total-energy curve symmetric with respect to a change of the sign of  $\theta$ . This means an extremum of the total energy for the ferromagnetic configuration,  $\theta=0$ , is predetermined by symmetry. In the relativistic case, however, the total energy as a function of  $\theta$  is not symmetric about  $\theta=0$ . In fact, for reasons of symmetry no extremum of the total energy at  $\theta=0$  is expected. As a result, the position of the extremum of the the total energy curve as a function of  $\theta$  is "accidental" i.e. not determined by the symmetry of the problem.

The deviation of the magnetic moments from parallel directions in the case of  $U_3P_4$  which

are caused by symmetry properties of the crystal and magnetic structures reminds us of the effect of weak ferromagnetism in  $\text{Fe}_2\text{O}_3$ , connected with the names Dzialoshinski and Moriya. We therefore show in the next Sect. that our symmetry analysis together with the method of calculation also explains this interesting case.

## 6 First principles study of weak ferromagnetism in $\text{Fe}_2\text{O}_3$

The phenomenon of weak ferromagnetism has been known for more than forty years (see e.g. [25]). It is characterized by a small net magnetic moment resulting from a collection of atomic magnetic moments that nearly cancel each other, one of the best known examples being  $\alpha\text{-Fe}_2\text{O}_3$ . It has traditionally been discussed in terms of a model Hamiltonian of localized atomic moments of the form

$$H = I_{ij}\mathbf{S}_i\mathbf{S}_j + \mathbf{d}_{ij}[\mathbf{S}_i \times \mathbf{S}_j] + K_x S_x^2 + K_y S_y^2 + K_z S_z^2 \quad (9)$$

This Hamiltonian was suggested by Dzialoshinski [26] on the basis of phenomenological arguments. Moriya [27] showed that Dzialoshinski’s explanation can be given a microscopic footing by means of Anderson’s perturbation approach to magnetic superexchange. The first term of the Hamiltonian (9), the symmetric exchange, is supposed to lead to a compensated magnetic configuration. The next two terms, the anisotropic exchange and the magneto-crystalline anisotropy terms, respectively, can lead to a small ferromagnetic moment in an otherwise antiferromagnetic crystal.  $\alpha\text{-Fe}_2\text{O}_3$  is a classical example of a weak ferromagnet where the antisymmetrical exchange plays a key role.

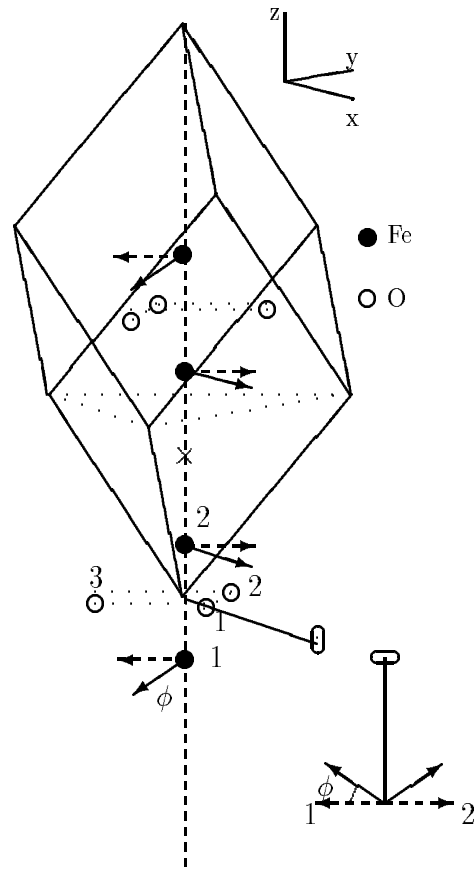
The unit cell of the  $\alpha\text{-Fe}_2\text{O}_3$  is shown in Fig. 4. We start our calculation with the magnetic moments of the Fe atoms directed along the y axis which corresponds to the experimental situation at temperatures below that where weak ferromagnetism occurs. As was discussed above, in the scalar-relativistic case any collinear structure will be stable during calculations. However with the spin-orbit coupling taken into account the magnetic moments start to move until that magnetic configuration is reached where the total energy is lowest. The directions of the moments thus calculated are shown in Fig. 4. by solid arrows. Canting of magnetic moments produces a small ferromagnetic component of about  $0.002 \mu_B$  per Fe atom. This estimate is in a quite good agreement with the experimental value. Our symmetry analysis easily explains this canting as follows. With the spin-orbit coupling taken into account only four symmetry operations are left in the group of the

FIG. 4 The unit cell of  $\text{Fe}_2\text{O}_3$ . Cross on the diagonal of the rhombohedron shows the point of inversion. The solid line passing through the first oxygen atom indicates a twofold symmetry axis. The collinear (dashed arrow) and canted (solid arrow) directions of the Fe atoms are shown. The canting of the Fe moments in the xy plane is demonstrated differently in the lower right corner of the Figure.

Kohn-Sham Hamiltonian: the identity transformation, the  $180^\circ$ -rotation about the x-axis and these operations multiplied by the inversion. Inversion transforms the atoms of the upper  $\text{Fe}_2\text{O}_3$  molecule into the atoms of the lower molecule, see Fig. 4 and, since the magnetic moments are axial vectors, they do not change under this transformation. Hence, the corresponding atoms of the two molecules must keep parallel moments and we may restrict our consideration to the lower molecule in Fig. 4. The only condition imposed on the moments of the Fe atoms by symmetry is the transformation of the moment of atom 1 into that of atom 2 by a rotation through  $180^\circ$  about the x-axis (see Fig. 4). However to fulfill this condition it is not necessary for the atomic moments to be parallel to the y-axis nor to remain collinear. Correspondingly, in the simulated annealing process, the magnetic moments deviate from their collinear initial directions toward the direction of the x-axis (see Fig. 4) until an “accidental” self-consistent magnetic structure preserved during iterations will be achieved.

An essentially different type of weak ferromagnetism was observed in  $\text{Mn}_3\text{Sn}$  [28]. Its magnetic structure is triangular and almost antiferromagnetic. A small canting of the magnetic moments leading to a weak ferromagnetic component cannot be caused in this case by the antisymmetric exchange because the contributions from different atoms cancel perfectly. Here the effect is supposed to be caused by the magneto-crystalline anisotropy. We carried out first-principles calculations [30] and obtained also in this case a very good description of the weak ferromagnetism. Again, in the scalar-relativistic calculation the ground state appears to be antiferromagnetic. But with spin-orbit coupling taken into account some magnetic moments deviate destroying the





complete magnetic compensation. Thus our method is universal and describes both types of weak ferromagnetism in the same calculational scheme.

## 7 Conclusion

In this short review we have shown that the local density approximation to density functional theory supplies a reliable basis for first-principles studies of non-collinear magnetic configurations in crystals. We restricted our discussion to ordered non-collinear structures which allowed us to use symmetry arguments to both, make accurate calculations possible and to render the physics transparent. We have shown that a consequent development of the density functional theory allows to explain within the itinerant electron picture the physical phenomena which were traditionally discussed in terms of the model Hamiltonian of localized moments.

The shortage of space did not allow us to discuss even briefly our work on an essentially different role of the spin-orbit coupling in non-collinear magnetism in various other U compounds [23]. Furthermore, we did not discuss calculations of the q-dependent magnetic susceptibility [22], nor the use of the methods of non-collinear magnetism to study effects of non-zero temperatures [6, 29] as well as the work of other groups like that of [4, 5, 11, 12, 13, 15, 16, 31] on different aspects of non-collinear magnetism. Neither could we give a reasonably complete list of references to the work of others. Still we hope to have succeeded in giving an impression of the present state of the local density functional theory of non-collinear magnetism and supply at least a few first references for those who will want to gain a deeper insight into this rapidly developing branch of the physics of itinerant magnetism.

**Acknowledgment** This work benefited very much from the help and cooperation of M. Uhl; it was supported by the SFB 252 Darmstadt, Frankfurt, Mainz. It also benefited from collaboration within the European Union's Human Capital and Mobility Network on "Ab-initio (from electronic structure) calculation of complex processes in materials" (contract: ERBCHRXCT930369)

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# Network Conference

organized by the European Union HCM network

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

**Schwäbisch Gmünd, Germany  
September 17-21, 1996**

*Third Circular, call for abstracts and  
Applications for financial support  
Deadline: May 25<sup>th</sup>*

*Hotel Reservations and Registration  
Deadline: July 1<sup>st</sup>*

## **PRELIMINARY PROGRAM** (not confirmed by all invited speakers)

**TUESDAY Sept 17**

17.00-20.00 Registration

### WEDNESDAY Sept 18

8.00 - 8.45	Registration		
8.45 - 9.00	Welcome		
9.00 - 9.55	M Parrinello		
	O(N)-1:	DF-1:	P&MT-1:
10.00-10.30	Coffee	M Pederson	D Singh
10.30-11.00	W Kohn	Coffee	P Blöchl
11.00-11.30	M Gillan	A Svane	Coffee
11.30-12.00	2c	2c	2c
12.00-12.30	2c	2c	2c
	O(N)-2:	DF-2:	P&MT-2:
14.00-14.30	D Pettifor	E K U Gross	F Gygi
14.30-15.00	P Ordejon	T Kotani	2c
15.00-15.30	I Abrikosov	Coffee	2c
15.30-16.00	Coffee	F Aryasetiawan	2c
16.00-16.30	2c	M Rohlfing	Coffee
16.30-17.00	2c	2c	O Jepsen
17.00-17.30	2c	2c	R Zeller
17.30-18.00	2c	2c	2c
19.00-	Food and Posters		

### THURSDAY Sept 19

8.30 - 9.25	O Eriksson		
	DF-3:	MD-DF:	OTHER:
9.30-10.00	P Oppeneer	N Marzari	2c
10.00-10.30	A Liechtenstein	Coffee	2c
10.30-11.00	F Manghi	P Ballone	Coffee
11.00-11.30	Coffee	2c	2c
11.30-12.00	2c	2c	2c

	QMC:	MAGN-1:	SEMIC-1:
14.00-14.30	L Mitas	S Blügel	J Neugebauer
14.30-15.00	2c	2c	2c
15.00-15.30	M Foulkes	B Ujfalussy	Coffee
15.30-16.00	O Gunnarsson	Coffee	P R Briddon
16.00-16.30	Coffee	2c	R Nieminen
16.30-17.00	2c	2c	2c
17.00-18.00	Posters		

### FRIDAY Sept 20

8.30- 9.25	P Bruno		
	MAGN-2:	C STRUCT:	SEMIC-2:
9.30-10.00	J Kudrnovsky	A de Vita	S Ossicini
10.00-10.30	K Schep	M Heggie	Coffee
10.30-11.00	Coffee	Posters	Posters
11.00-11.30	Posters	Coffee	2c
11.30-12.00	I Solovyev	2c	2c
	MAGN-3:	SURF&INF-1:	ORGANIC:
14.00-14.30	2c	S Wilke	J-L Bredas
14.30-15.00	2c	2c	2c
15.00-15.30	Coffee	H Joensson	G Brocks
15.30-16.00	Posters	Coffee	W Andreoni
16.00-16.30	P Carra	Posters	Coffee
16.30-17.00	H Ebert	P Feibelman	Posters
17.00-17.30	2c	2c	2c
17.30-18.00	2c	2c	2c
	MAGN-4:	SURF&INF-2:	CLUSTER:
20.30-21.00	M Stocks	A Gross	J Pacheco
21.00-21.30	B Harmon	2c	2c
21.30-22.00	2c	2c	2c

## SATURDAY Sept 21

8.30- 9.25	B Györfy		
	SUPERC:	SURF&INF-3:	CHEM R:
9.30-10.00	W Pickett	A Ruban	R Shah
10.00-10.30	S Savrasov	Coffee	2c
10.30-11.00	2c	E Tosatti	Coffee
11.00-11.30	Coffee	H Rücker	A Savin
11.30-12.00	2c	2c	2c
12.00-12.30	2c	2c	2c
	MAGN-5:	SURF&INF-4:	PHASE T:
14.00-14.30	M Fähle	M Finnis	I Mazin
14.30-15.00	2c	2c	2c
15.00-15.30	Coffee	B Hammer	D Vanderbilt
15.30-16.00	J Kübler	Coffee	2c
16.00-16.30	R Lorenz	J Dabrowski	Coffee
16.30-17.00	2c	A Fisher	2c
17.00-17.30	2c	2c	2c
17.30-18.00	SUMMARY: V Heine et al.		

2c = two contributed talks of 10+5 minutes  
Posters on exhibition for the entire duration of the Conference

## SYMPOSIA

### Methods

O(N)	Order N
DF	Density Functionals
P&MT	Pseudopotential and Muffin-Tin
QMC	Quantum Monte Carlo
MD-DF	<i>ab initio</i> Molecular Dynamics

## Applications

MAGN	Magnetism
SEMIC	Semiconductors
C STRUC	Carbon Structures
SURF&INF	Surfaces and Interfaces
ORGANIC	Organic Materials
CLUSTER	Metallic Clusters
SUPERC	Superconductors
CHEM R	Chemical Reactions (not at surfaces)
PHASE T	Structural Phase Transitions

## Attendance

The conference is open to anyone interested. The expected attendance is 300. Should the conference be overbooked, priority will be given according to time of registration.

## Contributed Talks and Posters

Any contribution within the field will be accepted, either as a 10 minute talk or as a poster, subject to the limitation that each participant presents at most one talk or poster. The author's preference, talk or poster, should be stated in the submitted abstract, but cannot be guaranteed. Note that a poster will be exhibited throughout the duration of the conference in the central foyer between the three lecture halls, where coffee will also be served. The slots allocated for contributed talks may be found in the Preliminary Program (2c).

## Abstracts – Deadline May 25<sup>th</sup>

Abstracts should be submitted as L<sup>A</sup>T<sub>E</sub>X files to [psik@radix2.mpi-stuttgart.mpg.de](mailto:psik@radix2.mpi-stuttgart.mpg.de).

The abstract format must follow the enclosed example as closely as possible. The name of the author presenting the contribution should be underlined (each author may present only one contribution). The book of abstracts will be handed out at the registration desk.

## Financial Support – Deadline May 25<sup>th</sup>

Limited funds are available for supporting active participation at the conference. The EU supports Network members. Members from associated nodes are supported directly by the respective country. Finally, we have asked the German Science Foundation (DFG) and the Max-Planck Society to support non-members, in particular younger scientists and scientists from Eastern Europe.

Applications from the associated nodes in Austria, Switzerland, Sweden or Finland should be directed to J. Hafner ([jhafner@email.tuwien.at](mailto:jhafner@email.tuwien.at)), P. Bloechl ([blo@zurich.ibm.com](mailto:blo@zurich.ibm.com)), B. Johansson ([sissela.uisk@Fysik.uu.se](mailto:sissela.uisk@Fysik.uu.se)) or R. Nieminen ([rniemine@csc.fi](mailto:rniemine@csc.fi)), respectively.

Other applicants should fill in the attached form and mail or fax it to O.K. Andersen. Applications received later than May 25<sup>th</sup> will not be considered. Answers will be e-mailed before June 15<sup>th</sup>. Reimbursement will take place at the conference and will require proof of actual travel expenses (e.g. train or plane ticket).

### **Registration – Deadline July 1<sup>st</sup>**

In order to attend the conference you must register by e-mail to [psik@radix2.mpi-stuttgart.mpg.de](mailto:psik@radix2.mpi-stuttgart.mpg.de). Furthermore a registration fee of DM 300.- must be paid upon arrival at the conference. This fee covers the costs of the facilities, the abstract booklet, morning and afternoon coffee and food at the poster evening.

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The enclosed hotel reservation card should be filled in and mailed to the tourist office (Verkehrsamt) in Schwäbisch Gmünd. Early reservation is advisable for nearby accommodation.

**Final Program** will be sent out in July.

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

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## **Further Information**

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

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## APPLICATION FORM

### Financial support for the participation at the $\Psi_k$ Network Conference 1996

(Not for associated members from Austria, Switzerland, Sweden or Finland)

Network Member: Yes [  ] No [  ]

If Yes: Node manager name \_\_\_\_\_ and signature \_\_\_\_\_

### Details about the Applicant

- Institution: \_\_\_\_\_
- City: \_\_\_\_\_ Country: \_\_\_\_\_
- Last name: \_\_\_\_\_
- First name, middle initial: \_\_\_\_\_
- Position: \_\_\_\_\_ Age: \_\_\_\_\_

### Applicant's conference contribution

- Symposium: \_\_\_\_\_
- Abstract title: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

For younger scientists: Supporting remarks from senior scientist in the field:

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### Travel Details

Travel from: \_\_\_\_\_ to Schwäbisch Gmünd by \_\_\_\_\_

Return to \_\_\_\_\_ by \_\_\_\_\_

Estimated transportation cost (cheapest fare): \_\_\_\_\_ DM

*We will reply via e-mail. Please print your full e-mail address below:*

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## Abstract submission example

### **L<sup>A</sup>T<sub>E</sub>X-Source:**

Note that the presenting author's name is underlined. The preferred symposium and mode of presentation are specified as comments at the beginning of the file.

```
%%%%%%%% Requested Symposium (from the 3rd circular): SUPERC
%%%%%%%% Preference (Talk or Poster): Talk
\documentstyle[]{article}
\begin{document}
\begin{center}
{\bf Quasiparticle bands and superconductivity in bilayer cuprates.}\[3mm]
\underline{A.I. Liechtenstein}, O. Gunnarsson, O.K. Andersen, and R.M. Martin\\
Max-Planck-Institut f\"ur Festk\"orperforschung,\\
Heisenbergstr.1, D-70569 Stuttgart, FRG
\end{center}
\begin{abstract}
We analyze the generic features of the energy spectrum
for two coupled CuO2 layers with a realistic extended Hubbard
model. The quasiparticle bands exhibit flat regions near X(Y) points
in the Brillouin zone with a large reduction of the
bonding-antibonding splitting, and pinning of extended
van-Hove singularity to the Fermi level, which is more efficient for
a bi-layers than for a single layer. In contrast to the results
with simpler models, the superconducting temperature
for dx2-y2 pairing is not lowered by the bi-layer hopping.
\end{abstract}
\end{document}
```

This would result in the following printout:

### **Quasiparticle bands and superconductivity in bilayer cuprates.**

A.I. Liechtenstein, O. Gunnarsson, O.K. Andersen, and R.M. Martin  
Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, D-70569 Stuttgart, FRG

#### **Abstract**

We analyze the generic features of the energy spectrum for two coupled CuO<sub>2</sub> layers with a realistic extended Hubbard model. The quasiparticle bands exhibit flat regions near X(Y) points in the Brillouin zone with a large reduction of the bonding-antibonding splitting, and pinning of *extended* van-Hove singularity to the Fermi level, which is more efficient for a bi-layers than for a single layer. In contrast to the results with simpler models, the superconducting temperature for d<sub>x<sup>2</sup>-y<sup>2</sup></sub> pairing is not lowered by the bi-layer hopping.