Ψ_k Newsletter

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

Number 26 April 1998

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

Contents

1 Editorial

In the section **News from the TMR1 Network** there is an announcement of the joint TMR1 Network and ESF Programme **Workshop on TB-LMTO**. There also the **Workshop on Spectroscopy** and the **2nd Annual Meeting** are announced. Please note, that apart from the general job advertisements in the usual place of the *Newsletter*, the TMR2-Network announces its positions in the section **News from the TMR2 Network**. In this section there is also some additional information on the **Industry Workshop**, jointly organized with the ESF Programme. The workshops and conferences organized outside the Psi-k Community Networks and Programmes are as usually advertised in the section on **General Workshop/Conference Announcements**. In the **Scientific Highlight** section we have an article by C. Blaas, L. Szunyogh, P. Weinberger, P.M. Levy, J. Banhart and C. Sommers on *'Electrical conductivity of multilayer systems'*. This highlight is reflecting one of many activities within the TMR1 Network on *'Interface Magnetism'*.

The *Networks* have a home page on World Wide Web (WWW). 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)*, *P. Blöchl (IBM, Zürich)*, *M. Gillan (Keele)*, *E.K.U. Gross (Univ. Würzburg)*, *B.L. Györffy (Bri stol)*, *V. Heine (Univ. Cambridge)*, *R. Jones (Univ. Exeter)*, *J. Kübler (TH, Darmstadt)*, *J.L. Martins (INESC, LISBON)*, *R. Nieminen (TU, Helsinki)*, *J. Nørskov (TU, Lyngby)* with information on CAMP, *M. Scheffler (FHI Berlin)*, *K.-H. Schwarz (TU, Vienn a)*, *G.P. Srivastava (Univ. Exeter)*, and *A. Walker (UEA Norwich)*. There are also pointers to the WWW home page of the Solid State Theory Group at National Renewable Energy Laboratory, Golden, CO 80401 *(http://www.sst.nrel.gov)*, and to the home page of Prof. David Vanderbilt, Department of Physics and Astronomy, Rutgers University *http://www.physics.rutgers.edu/ dhv.* If you maintain a home page on your activities we will be happy to include a pointer from the *Networks'* home page to your home page.

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

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

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

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

2 General News

The Psi-k Newsletter is the official communication and report vehicle for the TMR1 and TMR2 Networks and the ESF Psi-k Community. This is the main reason why it is divided into the separate sections dedicated mostly to those three European activities. Also, we like to think that it makes the reporting tidier. However, in practice there is so much overlap, because we are a one big electronic structure community. The scientific highlights are the highlights for the community as a whole. Therefore, we shall always welcome as many highlights as possible. There is no rule which says that we have to have just one scientific highlight per issue. We would like to encourage all our readers to submit to us all that would be of interest to the community as a whole. Of course, we are also very happy to publish in the Psi-k Newsletter any scientific and general information from outside the three networks, be it the conference/workshop or position announcements, scientific highlights and abstracts. We have the general sections specially designed for those purposes. As before, we would welcome reports on collaborative visits, workshops and conferences, and anything that can increase our scientific awareness in the field. Please share with us your opinion on the present outline of the Newsletters. It is in the interest of the whole community to make it as tidy and useful as possible.

3 News from the TMR1 Network

"Interface Magnetism"

There are three important meetings of this Network to take place within the next few months and their announcements are included below. Please note that the **Workshop on Spectroscopy** will take place very soon.

3.1 Workshop on Spectroscopy

Münich, 24-26 April, 1998

This workshop will bring together theoreticians from the TMR Network on **'Interface Magnetism'** and the experimentalists from the German Dichroism Network on **"Zirkular polarisierte Synchrotronstrahlung: Dichroismus, Magnetismus und Spinorientierung"**. This Workshop will give a good overview of the dichroism work on magnetic solids and multilayers. Anybody wishing to contribute please contact Hubert Ebert (he@gaia.phys.chemie.uni-muenchen.de).

3.2 2-nd Annual Meeting of the TMR1-Network

Begin: June 5, 1998, 14:00

End: June 7, 1998, 16:00

This annual meeting follows on from the successful meeting in Bristol last year which brought together 60 participants from the six nodes in Austria, France, Germany, Sweden, The Netherlands and UK.

As it is planned to have most contributions as regular (refereed) articles in a special issue of the Philosophical Magazine B, the following conditions and deadlines apply:

(1) Length of articles:

Latex standard version, article style, 12p, a4, textwidth 17.5cm, textheight 24.0cm:

5 pages maximum, including figures and references

(2) Dead-line for manuscripts: May 25, 1998

(3) Dead-line for manuscripts that have to be revised: July 1, 1998

These dead-lines have to be observed rigorously, since by July 6, 1998 all manuscripts have to be in the print shop at Taylor & Francis in London. PLEASE NOTE: ALL FINAL MANUSCRIPTS THAT ARE SENT AFTER July 1 WILL NOT BE IN THIS VOLUME!!!

(4) Manuscripts (Latex-file, postscript figures, British style of references!) should be sent to:

Peter Weinberger, e-mail: pw@cms.tuwien.ac.at

As a rule all contributions should be with respect to the 6 topics in the network:

(1) interlayer coupling,

(2) magnetic anisotropy and surface structure,

(3) Giant Magnetoresistance,

(4) spin-polarized spectroscopies,

(5) Tight-binding KKR-Green's function methods and

(5) Real space Tight-binding LMTO methods.

This special issue will then be the December 1998 issue of Phil. Mag. B.

In order to get an overview of possible contributions, attendance, abstracts etc., please reply as soon as possible, but at the latest of March 23, 1998 to

W. Temmerman, e-mail: W.M.TEMMERMAN@dl.ac.uk

and

P. Weinberger, e-mail: pw@cms.tuwien.ac.at

3.3 Workshop on the TB-LMTO Method

Monastery of Mont Saint Odile - France (one hour drive from Strasbourg)
2-5 October 1998

Supported by TMR * "Interface Magnetism" and ESF**
Program STRUC (Electronic Structure Calculations for elucidating the complex atomistic behaviour of solids and surfaces)

MOTIVATION

In recent years, computational materials science has clearly emerged as an important field in its own right. It is now well established that methods based on a microscopic description of the electronic structure are central points. In order to describe always larger systems, localized orbitals approaches are very useful. The TB-LMTO (Tight-Binding Linear Muffin-Tin Orbitals) method combines the precision of the ab-initio methods and the flexibility of the tight-binding schemes. The always increasing facilities provided by the supercomputers has for good shown the interest of the order N methods. For thoses reasons the TB-LMTO is widely used to study many different problems. This workshop intends to allow a large meeting of scientists involved in the development and the use of this method. The workshop will focus on the magnetic properties but other field of applications will be considered

SCOPE

The workshop will have two parts. The most important one will be devoted to invited talks where speakers will be asked to present the fundamental aspects of the problems. In a second part applications of this method will emphasize the interest of the method.

Aspects to be covered include:

- - Full Potential approaches
- - Relativistic DFT
- - Toward an Implementation of Relativistic DFT
- - Magnetic anisotropy
- - Non-collinearity
- - Alloy: CPA-TB-LMTO
- - Magnetic Interlayer coupling
- - Surface segregation and Surface roughness
- - Spectroscopic aspects

- - Response function
- - Recursion method
- - Latest developments of order(N)
- - Large systems studies
- - Sparse matrix techniques

The invited speakers are (20/3/98): I. Abrikosov (Uppsala), O. Andersen (Stuttgart), M. Alouani (Strasbourg), H. Ebert (Munich), O. Eriksson (Uppsala), J. Hafner (Vienna), D. Stoeffler (Strasbourg), I. Turek (Brno), W. Temmerman (Daresbury) and J. Wills (Los Alamos).

To be confirmed: I. Duff (RAL, Daresbury), J. Kudrnovsky (Praha), M. Methfessel (Frankfurt/Oder) and H. Skriver (Aarhus)

A large number of PhD students or post-docs are expected to participate. Financial support of the TMR network " Interface Magnetism" and hopefully of the ESF program STRUC could be provided to elegible persons. The total number of participants should not go beyond sixty.

PUBLICATION

We intend to publish a book about the TB-LMTO method, giving all basic aspects of this method (which now can be found only in specialised publications) and few applications.This book will consist of selected contributions to this workshop and have around 300-350 pages.

PREREGISTRATION

I would like to be informed on this TB-LMTO workshop; YES - NO
I intend to participate to this TB-LMTO workshop: YES - NO
I intend to present a contribution (tentative title):

Name, Last name:
Address:
Tel:
Fax:
E-mail:

ORGANIZATION

Hugues Dreyssé
IPCMS-GEMME, Université Louis Pasteur,
23 rue du Loess,

BP 20 CR,
67037 Strasbourg, France.
Tel.: +33/ 388.10.70.83
Fax: +33/ 388.10.72.49
E-mail: hugues@lugh.u-strasbg.fr

* Training and Mobility Research, a European network sponsored by the EC.

** European Science Fundation (support to be confirmed).

4 News from the TMR2 Network

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

The TMR2 network started on March 1, as anticipated. It has got a homepage, which you might consult for a detailed description of its scientific programme, planned future activities and vacant positions:

http://da601.dfi.aau.dk/ svane/tmr-psik.htm

The first very important activity of this Network is the **Industry Workshop** which we write about below. This Workshop is our big exercise of reaching out to industry to establish common projects. Therefore it should be in the iterest of all of us to ensure that our industrial partners are aware of this meeting and contribute with their talks.

Network Coordinator
Axel Svane
svane@dfi.aau.dk

4.1 Industry Workshop

Vienna, June 3-4, 1998

Sponsored by TMR2-Network and the ESF Programme

This workshop is seeking contributions, from Industry and Academia, of *'Ab initio electronic structure calculations for chemical/petrochemical/pharmaceutical industry, electronic industry, structural materials and magnetic materials'*. So far, presentations will be given by speakers from the following companies: Institut Francais du Petrole, Total, Basf, Rhone-Poulenc, DSM, Topsoe.

For further information please contact Erich Wimmer at:

ewimmer@msi.fr

Post-doctoral Position

Condensed Matter Theory: Electronic Structure of f-electron materials

Institute of Physics and Astronomy,
University of Aarhus, Denmark

Applications are invited for a post-doctoral position funded by the European Training, Mobility and Research Network, **Psi-k**:

'*Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Science*'

The position is available for a period of 2 years starting 1st of April 1998 or later.

The applicant is expected to contribute to the network project on investigations of f-electron systems based on the self-interaction corrected version of density functional theory. This implies applications of present computer codes to lanthanide and actinide systems as well as development of improved computer codes. The project is a collaboration in an international team, comprising research groups in Aarhus, Daresbury, Dresden and Uppsala. Some travel activity between the research centers involved must be foreseen. More detailed information concerning the project can be obtained upon request.

The applicant should hold a PhD degree or equivalent in Physics or Chemistry, be younger than 35, and should have some experience in computational Condensed Matter Theory. He/She must be of European Union nationality (or from Norway, Iceland, Israel, or Liechtenstein), however excluding Danish residents.

The salary will be around 25.000 DKr, but due to be taxed. Count on appr. half this amount in your hand.

Please, send inquiries and applications to:

Dr. A. Svane
Institute of Physics and Astronomy
University of Aarhus
Ny Munkegade
DK-8000 Aarhus, Denmark

Tel.: (+45) 8942-3678
Fax.: (+45) 8612-0740
Email: svane@dfi.aau.dk

Post-doctoral Position at MSI in France

A post-doctoral position in the area of electronic structure theory of surfaces is available at Molecular Simulations (MSI) in Orsay, France. This three-year position is supported by the European Ψ_k Network and is part of the programme for Training and Mobility of Researchers (TMR). The research area will include the study of the structural and electronic properties of metal oxide surfaces, in particular those of $Fe2O_3$ and Fe_3O_4, an investigation of the catalytic reaction of ethylbenzene to styrene, and the role of surface defects.

Candidates should have experience with density functional methods such as the pseudopotential plane wave methods and all-electron localised orbital methods. Experience with surface electronic structure calculations and catalytic systems are desirable.

The position would be based in the French offices of Molecular Simulations, which are located near Paris in Orsay. In the spirit of the TMR2 Network, the position would also provide for visits to the research groups of the other members of the network in Germany, the UK, Greece, and other European countries.

Candidates from European Union (or from Norway, Iceland, Israel, and Liechtenstein), excluding France, should send their applications before March 31 to:

Erich Wimmer
Molecular Simulations
Parc Club Orsay Universite
20, rue Jean Rostand
91893 Orsay, France
Tel: +33 1 69 35 32 27
Fax: +33 1 69 41 99 09
E-mail: ewimmer@msi.fr

POST-DOCTORAL POSITION

Computational Condensed Matter and Materials Physics

Laboratory of Physics, Helsinki University of Technology

Applications are invited for a post-doctoral position funded by the European Training, Mobility and Research Network

"Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Science" (Psi-k)

The position is available for a period of 2 years starting 1st of April 1998 or later.

The applicant is expected to contribute to the network project on investigations of excited-state and nonequilibrium properties based on extensions of density-functional theories. This includes development of improved computer codes as well as applications to optoelectronic properties of novel semiconductor materials and quantum structures. The project is a collaboration in an international team, comprising research groups in Helsinki (Espoo), Aarhus, Paris and Würzburg. Some travel activity between the research centers involved must be foreseen. More detailed information concerning the project can be obtained upon request.

The applicant should hold a Ph. D. degree or equivalent in Physics or Chemistry, be not older than 35, and should have some experience in computational condensed matter theory.

He/She must be of European Union nationality (or from Norway, Iceland, Israel, or Liechtenstein), however excluding Finnish residents.

The net salary will be around 11500 FIM per month after taxes. There will also be contributions towards relocation and travel costs.

The research group at HUT includes presently two senior faculty, six post-docs and visitors and fifteen doctoral students. It has excellent facilities for large-scale computational and theoretical research.

Please, send inquiries and applications to:

Prof. Risto M. Nieminen
Laboratory of Physics
P.O. Box 1100
02015 HUT
Finland

tel.: +358-9-451 3105
fax: +358-9-451 5067
email: rniemine@csc.fi

POST-DOCTORAL POSITION AT WÜRZBURG UNIVERSITY

Applications are invited for a 2-years postdoctoral position in the area of electronic structure theory of superconductors.

The position is funded by the European psi-k network as part of the programme for Training and Mobility of Researchers (TMR).

The applicant will be involved in first-principles electronic-structure calculations of the superconducting state of matter. The aim is to predict materials-specific properties of superconductors, including the High-Tc compounds, on the basis of the density functional theory for superconductors. The project includes the development of new exchange-correlation functionals and the investigation of relativistic effects in superconductors.

The candidate should have profound experience with Kohn-Sham-based band-structure calculations. Besides that, knowledge in the field of superconductivity will be most welcome.

The position will be based at the Institute for Theoretical Physics of the University of Wurzburg, Germany. The project is carried out in close collaboration with research groups at the University of Bristol, the Max-Planck-Institute for Solid-State Research in Stuttgart and the Daresbury Laboratory. Several visits to these reseach centres are anticipated.

Due to TMR regulations, the candidate must be of EU nationality (or from Iceland, Israel, Liechtenstein or Norway) excluding, however, German nationals and EU nationals who have resided in Germany for more than 6 months during the past 2 years. The applicant should not be older than 35.

Interested individuals should send their appication before May 31 to:

Prof. E.K.U. Gross
Institut für Theoretische Physik
Universität Würzburg
Am Hubland
D-97074 Würzburg
Germany

Phone: ++49-931-888-5724
Fax: ++49-931-888-5141
E-mail: gross@physik.uni-wuerzburg.de

5 News from the ESF Programme

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

The contract with the ESF regarding the Psi-k ESF Programme have now been finalised. This means that the Psi-k collaborative visits programme has been restarted. The rules of applying for financial support to make a collaborative visit between different scientific institutions in Europe are the same as in the case of the former HCM Ψ_k-Network. One simply needs to submit a small scientific proposal, with an estimate of costs involved, to **psik-management@dl.ac.uk**. The decision approving the visit will be taken within two weeks from submission of the proposal. Please note that only the scientists from the countries which contribute to the Psi-k ESF Programme can benefit. They are: Austria, Belgium, Denmark, Finland, France, Germany, Hungary, Ireland, Italy, Poland, Portugal, Slovenia, Sweden, Switzerland and UK.

An important event of the ESF Psi-k Programme is the **Industry Workshop** in Vienna on June 3-4, 1998. This workshop is jointly sponsored by the ESF and the TMR2. More details are to be found in the preceding section dedicated to **News from the TMR2 Network**.

The steering committe of the ESF programme will hold its inaugural meeting during the **Industry Workshop** in Vienna on June 3-4, 1998. The commitee consists of the following Ordinary Members: Belgium: Vic Van Doren (Flemish Community) and Jean-Pol Vigneron (French Community), Denmark: Axel Svane, Finland: Risto Nieminen, France: Hugues Dreysse, Germany: Stefan Blugel, Hungary: Janus Kollar, Ireland: Charles Patterson, Italy: Raffaele Resta, Poland: Adam Kiejna, Portugal: Jose-Luis Martins, Slovenia: Ales Zupan, Sweden: Olle Eriksson, Switzerland: Rene Monnier, UK: Mike Finnis. The Chairman is Volker Heine, the Acting Chairman is Juergen Hafner and the Secretary is Walter Temmerman. In addition, to the above Ordinary Members, the following scientists may be invited as Advisory Members of the Steering Committee: Ole Andersen (D), Olmes Bisi (I), Peter Dederichs (D), Paul Durham (UK), Mike Gillan (UK), Hardy Gross (D), Balazs Gyorffy (UK), John Inglesfield (UK), Christiane Koenig (F), Jens Norskov (DK), Jose Ortega (E), Matthias Scheffler (D), Dzidka Szotek (UK) and Erich Wimmer (F).

This meeting will consider four proposals for workshops in 1998: Nanotechnologies (Andrew Fisher), Minerals (Juergen Winkler), Local Orbitals (Pablo Ordejon), TB-LMTO (Hugues Dreysse). Moreover, one proposal for a workshop in 1999 has been received from Bob Jones on Hydrogen in Semiconductors.

6 General Workshop/Conference Announcements

6.1 CAT98 - 2nd Announcement

and
Call for Abstracts

7th International Conference on Theoretical Aspects of Heterogeneous Catalysis

Downing College, Cambridge, UK
25th-28th August 1998

SPONSORED BY: Hamilton Systems, ICI Katalco, Johnson Matthey PLC, Molecular Simlulations Inc, Olivetti Research

BURSARIES FOR YOUNG SCIENTISTS

Following support from the EC TMR Programme, bursaries are available to qualifying scientists who are under 35.

OLIVETTI RESEARCH PRIZES for the best talk and the best poster by a graduate student.

Local Organizing Committee: DA King, A Wander, RM Lambert, M Payne, NC Handy, DJ Wales

International Scientific Committee: EJ Baerends, PS Bagus, DM Bird, CRA Catlow, G Ertl, MJ Gillan, S Holloway, F Illas, BI Lundqvist, M Neurock, C Noguera, JK Norskov, G Pacchioni, TA Pakkanen, C Pisani, N Rosch, J Sauer, P Sautet, and M Scheffler

INVITED SPEAKERS:

F. Besenbacher (*University of Aarhus*) "Dynamics of diffusion, adsorption and reactions on metal surfaces studied by STM"

E.A. Carter (*University of California at Los Angeles*) "Ab initio CI/DFT embedding theory of chemisorption on metals and metal oxides"

C.R.A. Catlow (*The Royal Institution of Great Britain*) "Modelling of diffusion and reactivity in microporous materials"

M.J. Gillan (*Keele University*) "The systematics of acid-base reactions on oxide surfaces: insights from first-principles calculations"

Y. Inoue (*Nagaoka University of Technology*) "Accoustic wave effects on activity and selectivity of thin film catalysts combined with ferro-electric substrates"

C. Noguera (*The University of Paris-Sud*) "Electronic processes on polar and non-stoichiometric oxide surfaces"

J.K. Norskov (*Technical University of Denmark*) "Dissociation and further reation of CO, NO

and N2 on transition metal surfaces"

S.M. Roberts (*University of Liverpool*) "Use of natural and non-natural biocatalysts in the prepararion of optically active pharmaceuticals"

N. Rosch (*Technical University of Munich*) "Metal species at ionic substrates (oxides and zeolites)"

A. Selloni (*University of Geneva*) "Adsorption of molecules and clusters at oxide surfaces"

E. Tossati (*University of Trieste*) "Simulations of adsorption-induced deconstruction"

J.L. Whitten (*North Carolina State University*) "Catalytic and photochemical reactions on Pt and Ni surfaces"

M. Wolf (*Fritz-Haber Institute, Berlin*) "Ultrafast surface dynamics of electrons and individual molecules"

TOPICS

The conference will cover the following topic areas.

Metallic Systems	Bimetallic Systems
Zeolites	Oxides Sulphides and Ionic Surfaces
Molecular Simulations and Dynamics	Supported Metals and Nanoparticles
New Directions	

Contributions on these, or other related topics are welcomed. Participants can apply to make an oral contribution or to display a poster.

ABSTRACTS

These should be one page of A4 with 25mm margins all round. Please use Times Font size 12 double spacing. Diagrams are permited but no colour.

DEADLINES

Deadline for Abstracts: 30th April 1998

Deadline for Registration: 15th June 1998

Your abstract will be acknowledged within one week of receipt. Registration forms should be returned as soon as possible to secure a young scientist's bursary. These will be offered on a first come first served basis and payment of the registration fee (minus bursary amount) must be received before 15th June in order to confirm this bursary.

TRAVEL INFORMATION

Air - Cambridge has its own airport,but with very limited international flights. Otherwise Stansted Airport is recommended. There is a regular coach service from all 3 London Airports to Cambridge (Gatwick 3+ hrs, Heathrow 2 hours, Stansted 30 minutes) Gatwick and Heathrow are also accessible by train . Downing College is 5 minutes walk from the Central Coach Station, but arrival by train or at Cambridge Airport would necessitate a bus or taxi journey. The Railway Station is 5-10 minutes by bus from Downing College. Car Parking is available at Downing College.

The first session of the meeting will be after lunch on 25th. The last session is on the morning

of 28th.

For Further information please e-mail: CAT98@ch.cam.ac.uk or write to: Sue Free, CAT98, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK.

CAT98 Website - **http://www.ch.cam.ac.uk/misc/cat98.html**
The 2nd Announcement and all future information including registration forms is available at this address.

REGISTRATION FORM

Personal details

Name:

Place of Work:

Address:

e-mail Addrress[1]:

Male/Female

Registration Fee ... (please tick as appropriate)

The registration fee includes 3 nights accommodation (25th, 26th and 27th), all meals and refreshments during the conference, starting with lunch of 25th, and the conference dinner on 27th. (Lunch will not be available at Downing College on 28th) Non-residents fee includes dinners as well as lunch, but not breakfast.

Resident Fee £260-00
Non Resident Fee (including all meals) £175-00
Special Dietary needs
(Please Specify)

Young Scientists
Are you entering for the Olivetti Prize as a registered student[2] ?

100 bursaries of £100-00 each are available on a first come first served basis to assist young scientists from the EU with attendance at the conference. Do you wish to apply for a bursary[3]?

Presentation

Would you prefer:
Oral Presentation
Poster
Neither

[1]IMPORTANT:- Communications concerning CAT98 will be conducted via e-mail

[2]Please enclose a letter of confirmation from your supervisor

[3]To qualify you must be an EU citizen (or associate states) and aged under 35. Please include a photocopy of your passport for confirmation.

6.2 EPS Conference-CMD17

Grenoble, August 25-29, 1998

THE 17TH GENERAL CONFERENCE OF THE CONDENSED MATTER DIVISION OF THE EUROPEAN PHYSICAL SOCIETY (CMD17) and LES 6EMES JOURNEES DE LA MATIERE CONDENSEE DE LA SOCIETE FRANCAISE DE PHYSIQUE (JMC6) to be held in GRENOBLE August 25-29 this year, are raising more and more interest. Over 3000 contacts, already, have reached our web server

http://www.polycnrs-gre.fr/eps.html

where the information was recently reactualised. In particular the time schedule of the scientific programme is included as well as the list of the plenary speakers. An additional minicolloquium (39 "NEW RESULTS IN CONDENSED MATTER") has been created to collect all important new developments in fields not properly covered by the former list. Consult our WEB server for additional information.

The incoming IMPORTANT DEADLINE for ABSTRACT submission and student's GRANT request is MARCH 15th. Other important deadlines are:
APRIL 15 – acceptance
MAY 15 – early registration.

6.3 First International Euroconference on Anomalous Complex Superconductors

Crete, Greece, September 26 - October 3, 1998

Updated information in the WEB:

http://www.physics.uch.gr/ acs1/

DEADLINES

Abstracts for contributed talks and posters before May 1, 1998.
Applications for financial aid to young European Union nationals (under 35) before May 1, 1998.
Applications for financial aid to East Europeans (few INCO grants are available) before May 1, 1998.
Notification of acceptance will be mailed by May 29, 1998.

All informations is in the above mentioned WEB page.

PROGRAM COMMITTEE

J. Fink (IFW-Dresden)
P.B. Littlewood (Cambridge)
D. van der Marel (Groningen)
H.R. Ott (ETH-Zuerich)
D. Schweitzer (Un. Stuttgart)
G. Varelogiannis (Heraklion)
D. Vollhardt (Augsburg)

PRELIMINARY LIST OF CONFIRMED SPEAKERS:

G. Aeppli (NEC-Princeton)
H. Alloul (Orsay)
J. Annett (Bristol)
M. Cardona (MPI-Stuttgart)
S.-L. Drechsler (IFW-Dresden)
O. Fischer (Geneva)
L. Greene (Urbana)
W. Hanke (Wuerzburg)
D.C. Johnston (Ames)
P. Kes (Leiden)
K. Kitazawa (Tokyo)
P.A. Lee (MIT)

G. Lonzarich (Cambridge)
J. Loram (Cambridge)
S. Maekawa (Sendai)
K. Maki (USC)
J. Mannhart (Augsburg)
A.J. Millis (John Hopkins)
J. Sauls (Northwestern)
Z.-X. Shen (Stanford)
S. Tajima (ISTEC-Tokyo)
Y. Tanaka (Niigata)
T. Timusk (McMaster)
P. Woelfle (Karlsruhe)
J. Zaanen (Leiden)

FURTHER INFORMATION

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acs1@physics.uch.gr

7 General Job Announcements

INSTITUTE OF PHYSICS AND ASTRONOMY UNIVERSITY OF AARHUS DENMARK

ASSOCIATE PROFESSOR IN CONDENSED MATTER THEORY

Applications are invited for a position as associate professor in condensed matter theory at the Institute of Physics and Astronomy. The position is open from October 1, 1998.

The successful applicant should strengthen the research in condensed matter physics at the Institute and complement the existing theoretical research, which includes activities in pattern formation and critical phenomena and in electronic structure theory. He/she should also contribute to teaching at the Institute at both the undergraduate and graduate levels.

The Faculty of Science specifically encourages younger candidates to apply with a view towards increasing the proportion of younger professors.

Research at the Institute covers atomic, condensed matter, nuclear and particle physics as well as astrophysics. Additional information about the Institute can be found at http://www.dfi.aau.dk/ or be obtained from the Head of the Institute, professor I. Stensgaard, Tel. +45 8942 3715, Fax: +45 8612 0740 or e-mail: fysis@dfi.aau.dk.

Applications should include a curriculum vitae giving evidence on which the evaluation of the applicant's scientific and teaching qualifications can be based, a complete list of publications together with three copies of each of those publications which the applicant selects as the most relevant for the application. Other supportive material should also be submitted in three copies.

The selection committee may include further material from the list of publications in its evaluation of the applicant. In that case the applicant must, upon request, submit the material to the selection committee.

The selection committee's written evaluation of the applicants will be sent in full to all applicants.

Applications should be addressed to The Faculty of Science, University of Aarhus, Ny Munkegade, Building 520, DK-8000 Aarhus C, Denmark and marked 212/5-118.

The deadline for the receipt of all application material is May 18, 1998 at 12.00.

Group Leader
Materials and Molecular Modelling
The Division of Materials Science and Technology (MATTEK)
CSIR, Pretoria, South Africa

The CSIR is a uniquely South African organisation, committed to innovation. The Division of Materials Science and Technology (MATTEK) - one of CSIR's strategic units - develops, transfers and applies new, improved or adapted scientific and technological expertise in different classes of materials and chemical processes.

We currently have a vacancy for a

GROUP LEADER: Materials and Molecular Modelling.

The post will involve the development of MATTEK's new Atomistic and Molecular Modelling group and integrate it into our research projects across a broad range of materials (e.g. metals, ceramics and polymers) and chemical processes, by

- evaluating current projects for molecular modelling potential
- leading and supervising ongoing modelling activities
- promoting the group's activities internally and externally (industrial prospects)
- working collaboratively with the Materials Modelling Centre, University of the North

Applicants should have a Ph. D. in Chemistry (Chemical Engineering), Physics or Materials Science plus at least 3 years experience - preferably in industry (e.g. force-field and quantum mechanical methods). The position focuses on applying the range of computational techniques in solving industrial problems. Strong leadership, good communication skills (and fluency in English), initiative and vision, are required qualities.

This position is based at CSIR's Scientiae site, Pretoria (South Africa).

Applicants who meet the stated requirements, should send a comprehensive CV to:

Mrs Nonnie Brauckmann
CSIR - MATTEK
P O Box 395
PRETORIA 0001, South Africa
Fax No. +27 12 841-3287
E-mail: nbrauck@csir.co.za

Closing date: April 16, 1998

Post-doc Positions
Condensed Matter Theory Group at North Carolina State University

One or more postdoc and/or senior postdoc positions are becoming available with the Condensed Matter Theory group at North Carolina State University, beginning this summer and/or fall. Our main activities are centered on the application and development of electronic structure methods. Specific projects concern nanotube materials, wide gap semiconductors, and semiconductor surface problems. The primary tool of investigation is a real-space ab initio code implemented on massively parallel supercomputers. The ab initio calculations are complimented with classical Molecular Dynamics and kinetic Monte Carlo simulations as needed.

The ideal candidate should have significant experience with density functional theory and quantum molecular dynamics calculations. He/she would be joining a large and very active group headed by Profs. Bernholc and Roland, and would be involved in a number of diverse and challenging research projects.

Interested persons should send their resumes and the names of references, preferably via email, as soon as possible. If practical, we would like to meet and/or interview interested candidates during the upcoming APS March meeting.

Please pass this message on to anyone you would consider appropriate. Thank you very much for your help.

Jerry Bernholc,
Email: bernholc@ncsu.edu,
Phone: (919) 515-3126,
Secretary: (919) 515-3468

Chris Roland,
Email: roland@ajax.physics.ncsu.edu;
Phone: (919) 515-3170,
Secretary: (919) 515-3468

Department of Physics,
NC State Univ.,
Raleigh, NC 27695-8202
FAX: (919) 515-7331

Postdoctoral Position in Solid State Theory Group

National Renewable Energy Laboratory

http://www.sst.nrel.gov

The Solid State Theory Group at the National Renewable Energy Laboratory invites applications for postdoctoral research positions. The positions are for two years, renewable upon mutual agreement to a third year. The general research areas involved are (i) semiconductor nanostructures and (ii) alloy theory. The Solid State Theory Group currently consists of ten Ph.D.'s in condensed matter theory (including Drs. Alex Zunger, Su-Huai Wei, and Chris Wolverton) and interacts with a broad range of experimentalists at NREL. For more information about group research activities, see http://www.sst.nrel.gov, and for more information about postdoctoral positions, see http://www.sst.nrel.gov/postdoc/postdoc.html. The theory group is a renowned research group with an outstanding record of publication and innovation. Furthermore, the group has outstanding computational facilities, an excellent basic-research atmosphere, and is located in the beautiful Rocky Mountains (less than one hour from hiking and ski resorts). Interested candidates should immediately send in writing a curriculum vitae, list of publications (including preprints of unpublished papers, if possible) and list of two references, addressed to:

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

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

Post-Doc Position

Condensed Matter Theory
University of Missouri-Columbia

I would appreciate if you could bring the following open post-doc position to the attention of anyone who might be interested. I apologize if you received this twice or if you shouldn't have received this message in the first place.

A post-doctoral position is available in the general area of electronic structure of solids beginning Summer or Fall 1998. The position is available for one year and may be extended for up to two years subject to availablility of funding. Main activities of my group are centered on Density-Functional Calculations and Study of models extracted from such calculations using both computational and analytical tools as appropriate.

Currently, we are working on a number of problems on the Colossal-MagnetoResistive (CMR) oxides including DFT Calculations, Study of Charge and Orbital ordering, Magnetic Exchange Mechanisms, Lattice and Spin polaron effects, Jahn-Teller couplings, etc. Quantum Molecular Dynamics and Monte Carlo calculations as applied to these and other systems are also of some interest. The ideal candidate should have good analytical and computational skills. Prior experience in density-functional calculations is not necessary. The work atmosphere is pleasant and strongly interactive. The group consists of typically two graduate students, one post-doc, and myself. The University of Missouri-Columbia has about 20 faculty members and 40 graduate students, about two thirds of whom are in condensed matter physics.

Interested persons should send their resumes and the names of references as soon as possible. If possible, I would like to meet and/or interview interested candidates during the upcoming APS March meeting in Los Angeles.

Sashi Satpathy
Assoc. Professor, Department of Physics
University of Missouri,
Columbia, MO 65211, USA
E-mail: satpathy@agni.physics.missouri.edu
Tel: (573)-882-4838 (Work)
FAX: (573) 882-4195(Work)

Post-Doc Position

Department of Physics, University of Rhode Island

We have a postdoctoral position available for work on Monte Carlo computation of eigenvalues in problems in statistical mechanics (critical phenomena) and quantum mechanics (van der Waals clusters). Please see `http://www.phys.uri.edu/~nigh/publications.html` for more details and references.

I would appreciate it if you would bring this to the attention of suitable candidates. I shall be at the APS March meeting and would like to meet there with anyone who is intested.

Peter Nightingale
Department of Physics, East Hall
University of Rhode Island
Kingston, RI 02881

Email: nigh@phys.uri.edu
Telephone: (401) 874-5882
Fax: (401) 874-2380

Post-Doctoral Position

Department of Physics, University of Bath, UK

Applications are invited for a post-doctoral research assistant funded by the UK Engineering and Physical Sciences Research Council to work on the project

"Theory of Promotion and Poisoning of Surface Reactions".

The post is available for three years, starting 1st April 1998, or as soon as possible after that date.

The aim of the project is to investigate the influence of pre-adsorbed species on the dissociative adsorption of molecules on metallic surfaces. First principles calculations, based on density functional theory, will be used to investigate the mechanisms underlying electronic promotion and poisoning effects in surface reactions. A key aim will be to use the results of large-scale calculations to break down the adsorbate-molecule interaction into direct interactions, substrate-mediated effects, electrostatic interactions, etc, and to hence develop semi-quantitative models of the strength and spatial range of promotion and poisoning effects.

Applicants should have, or expect soon to obtain, a PhD in Physics or Chemistry, with some experience in computational condensed matter theory. For further details please contact me by e-mail at the address given below.

Professor David Bird
Department of Physics
University of Bath
Bath BA2 7AY
United Kingdom
Tel: +44 1225 826586
Fax: +44 1225 826110
E-mail: d.bird at bath.ac.uk

Post-Doc Position

Department of Physics, University of Exeter, UK

A three year TMR postdoctoral position is available for work on Ab Initio Calculations for the Engineering of Defects in Advanced Semiconductor Devices.

This involves collaboration with, and visits to, groups in Sweden, Germany, Italy, Belgium, Denmark, Greece and the UK.

The postdoc will be involved with modelling studies aimed at understanding experiments carried out by members of the network. The position is subject to the regulations of the TMR programme and is available to non-UK European residents.

Details of the Training and Mobility of Researchers (TMR) programme can be found at:

http://www.cordis.lu/tmr/home.html

If you are interested, or know anyone who might be, please contact

R. Jones
Dept. of Physics,
University of Exeter,
Exeter EX4 4QL UK,
Email: r.jones@exeter.ac.uk
Fax: +44 1392 264111
Tel: +44 1392 264134

Ph. D. Position

Department of Physics, University of Exeter, UK

An EPSRC funded project studentship is available for work on 'Ab initio modelling of oxygen related defects in silicon'.

EPSRC has funded a three year study of Ab initio modelling of oxygen related defects in silicon. This work will link with experimental studies being carried out in the UK and Europe.

The student will receive the normal salary for a PhD student in the UK and all Ph. D. fees. The position is open to graduate students in Physics.

If you are interested, or know anyone who might be, please contact

R. Jones
Dept. of Physics,
University of Exeter,
Exeter EX4 4QL UK
email: r.jones@exeter.ac.uk
Fax: +44 1392 264111
Tel: +44 1392 264134

Industrial Post-Doc Position
Computational Solid State Chemistry
Norsk Hydro ASA, Norway

Industrial Post-Doc Position in Computational Solid State Chemistry Norsk Hydro ASA is Norway's largest industrial chemical group with more than 35000 employees world-wide. The central R&D facility is located in Porsgrunn with a staff of 430 people.

We are seeking for a Ph. D. level post-doc scientist to further strengthen our computational chemistry effort in the area of solid state chemistry.

The successful candidate will join a team of computational chemists which works on problems related to catalysis and polymers in close collaboration with experimental scientists.

The candidate should be a highly motivated, interactive and self-directing individual who will enjoy being an integral part of our research teams and is willing to take responsibility for the development and application of solid state modelling.

Background and experience in several of the following areas is desirable:

General solid state physics and chemistry background
Transition Metal Oxide Chemistry
Modelling Periodic Structures
Hartree-Fock
Density-Functional
Tight-Binding
Born-Shell Model
Ab initio MD
Program systems: Dsolid, CASTEP, CrystalXX, Unix, Fortran, C, C++

The Post-position is limited to one year but prolongation or permanent employment is not excluded.

If more information is desired, please contact Dr. Klaus Schöffel, phone: +47 35 56 4076, e-mail Klaus.Schoffel@hre.hydro.com, or Dr. Steinar Kvisle, phone +47 35 56 3463.

Applications marked "CONFIDENTIAL SS/98" should be sent as soon as possible to:

Norsk Hydro ASA
Research Centre Porsgrunn,
Personal Department,
P.O. Box 2560,
N-3901 Porsgrunn, NORWAY

8 Abstracts

Anisotropy energies and Heisenberg Hamiltonians

P. Weinberger
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Gumpendorferstr. 1a, A-1060 Wien, Austria

Abstract

Based on quite a general definition of anisotropy energies, namely as energy differences between two given magnetic configurations, "spin-flip" energies are defined in multilayer systems, which in turn can be mapped onto the parameters of a Heisenberg model, whereby the classical spin vectors pick up the meaning of orientations of the magnetization. By expanding the anisotropy energy in a series of the cosine of local rotation angles also continuous "spin-flip" energies can be formulated which then can be used to describe certain aspects of non-collinear magnetism. As will be shown the suggested model can easily be extended to "spin-spirals" and to the problem of domain walls. As an application results are shown for free and semi-infinitely capped surfaces of Fe on fcc Cu(100) and free surfaces of Fe on fcc Ag(100) by taking into account antiferromagnetic coupling between planes of Fe atoms.

(Submitted to Philosophical Magazine B)
Manuscripts available from: pw@cms.tuwien.ac.at

Magnetic anisotropy of Fe_xCo_{1-x} multilayers on Cu(001): reorientation transition of magnetic moments due to different interlayer coupling

J. Zabloudil[a], L. Szunyogh[a,b], U. Pustogowa[a],
C. Uiberacker[c], and P. Weinberger[a,c]
[a] *Center for Computational Materials Science, Vienna, Austria*
[b] *Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary*
[c] *Institut für Technische Elektrochemie, Technische Universität Wien, Vienna, Austria*

Abstract

The magnetic anisotropy energies of Fe_xCo_{1-x} multilayers on Cu(001) have been determined by means of ab-initio calculations using the fully relativistic, spin-polarized screened Korringa-Kohn-Rostoker method within the local spin density approximation. By utilizing the coherent potential approximation the Fe/Co system was treated within a mean-field approach as a (uniform) randomly disordered alloy. The type of magnetic interlayer couplings – either ferro- or antiferromagnetic – that is energetically more favorable, is found to depend on both the film thickness and alloy composition. Consequently, these parameters are responsible for the reorientation mainly because of the strong enhancement of the band energy contribution to the magnetocrystalline anisotropy energy in the case of antiferromagnetic couplings.

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

This paper resulted from a collaboration partially funded by the TMR network on 'Ab-initio calculations of magnetic properties of surfaces, interfaces, and multilayers' (Contract No. EMRX-CT96-0089).

Multiple reorientation transition of the magnetization of free surfaces of Fe on Ag(100)

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Institut für Technische Elektrochemie, Technical University Vienna, Austria
L. Szunyogh
Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary
and
Center for Computational Materials Science, Vienna, Austria

Abstract

The magnetic properties of Ag(100)/Fe$_n$, $n \leq 16$, are investigated using the fully relativistic spin-polarized Screened Korringa-Kohn-Rostocker method. It is found that (a) ferromagnetic interlayer coupling is the most stable magnetic configuration of free surfaces of Fe on Ag(100) and (b) that in the vicinity of $n = 5$ a multiple reorientation transition of the magnetization occurs. The results obtained are in excellent agreement with available experimental data and give an interesting explanation for the occurrence of temperature dependent effects seen experimentally.

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

This paper resulted from a collaboration partially funded by the TMR network on 'Ab-initio calculations of magnetic properties of surfaces, interfaces, and multilayers' (Contract No. EMRX-CT96-0089).

Spin-polarized X-ray emission spectroscopy of capped thin Co films on Cu(100)

U. Pustogowa[a], L. Szunyogh[a,b], H. Ebert[c], and P. Weinberger[a,d]
[a] *Center for Computational Materials Science, Gumpendorfer Str. 1a, A-1060 Vienna, Austria*
[b] *Department of Theoretical Physics, Technical University Budapest, Budafoki út 8, H-1521, Budapest, Hungary*
[c] *Institut für Physikalische Chemie, Universität München, Theresienstr. 37-41, D-80333 München, Germany*
[d] *Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Vienna, Austria*

Abstract

The theory of valence band X-ray emission spectroscopy (XES) is discussed in terms of spin-polarized fully relativistic multiple scattering. In comparison to the non spin-polarized case new theoretical features are presented with particular emphasis on the dependence of the intensity on the polarization of the emitted photon. In addition, the sensitivity of the spectrum to the relative angle between the directions of the emitted photon and the magnetization of a spectroscopically selected species is shown. Applications to the L_3 XES of a Co monolayer on Cu(100) substrate as capped by a monolayer of various $3d$, $4d$, and $5d$ transition metals are shown since such overlayer systems display systematic variations of the magnetic moment in the Co layer as well as in the cap layer. These changes are clearly mapped in the calculated XES and discussed in terms of transition cross sections and local densities of states.

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

This paper resulted from a collaboration partially funded by the TMR network on 'Ab-initio calculations of magnetic properties of surfaces, interfaces, and multilayers' (Contract No. EMRX-CT96-0089).

Effective Interatomic Interactions via the TB-LMTO Method

V. Drchal[a,b], J. Kudrnovský[a,b], A. Pasturel[c], I. Turek[d], P. Weinberger[b],
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[a] *Institute of Physics, Academy of Sciences of the Czech Republic,*
Na Slovance 2, CZ-180 40 Praha 8, Czech Republic

[b] *Institute for Technical Electrochemistry, Technical University of Vienna,*
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BP 166, 38042 Grenoble Cedex, France

[d] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic,*
Žižkova 22, CZ-616 62 Brno, Czech Republic

[e] *Lawrence Livermore National Laboratory, Livermore, CA 94550, U.S.A.*

Abstract

The energetics of metallic alloys, their surfaces or interfaces, and magnetic multilayers is studied in terms of the effective interatomic (or interlayer) interactions that are determined from ab initio electronic structure calculations using the TB-LMTO method combined with the coherent potential approximation and the method of surface Green functions. First the theoretical background (force theorem, Lloyd formula, generalized perturbation method for bulk and surfaces, vertex cancellation theorem, method of infinitesimal rotations) is discussed, and then the applications to the phase stability of bulk alloys, surface segregation in disordered alloys, magnetism-induced ordering in two- and three-dimensional systems, phase diagram of two-dimensional alloys, interlayer exchange coupling in metallic multilayers, and the construction of Heisenberg-like Hamiltonians for magnetic systems are presented.

(Submitted MRS Proceedings Fall Meeting 1997, Boston)
Manuscripts available from: pw@cms.tuwien.ac.at

Theoretical investigation of the high pressure phases of Ce

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[1] *Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, 75121, Uppsala, Sweden*
[2] *Center for Materials Science and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

Abstract

In order to shed light on the recent experimental controversy concerning the intermediate pressure phases of Ce we have made systematic electronic structure and total energy studies on Ce in the experimentally reported low pressure phase α-Ce (fcc), the intermediate pressure α-U (α'), the body centered monoclinic (α''(I)), and C-face centered monoclinic (α''(II)) phases, together with the stable high pressure body centered tetragonal phase. We also included the body centered cubic, hexagonal close packed and ω (hP3) phases. In this study we used the accurate full potential linear muffin-tin orbital method (FPLMTO). The optimized structural parameters obtained from our total energy studies for the α' and α''(II) phases are found to be in good agreement with corresponding experimental values. The structural optimization of the α''(I) phase always yields the fcc or bct phase stable, depending upon the volume considered. Except for an improvement in the equilibrium volume, the generalized gradient correction reproduces the calculated relative stability between different phases of Ce at high pressure of the local density approximation. Of the experimentally reported intermediate pressure structures (α', α''(I) and α''(II)) we find that the α''(II) phase is the most stable. Among the contending phases, α' and α''(I), the later is very close in energy whereas the former is substantially higher in energy. We thus rule out the α-U structure as an intermediate pressure phase of Ce. Our work suggests that the that the most probable structural phase transition sequence of Ce metal is fcc(γ) $\rightarrow$ fcc(α) $\rightarrow$ α''(II) $\rightarrow$ bct, which is consistent with current experimental results.

(Phys. Rev. B. **57**, 2091 (1998))
Preprints available from: ravind@fysik.uu.se

Reflectance Anisotropy of Silicon Surfaces: Discrete Dipole Calculation

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

Abstract

The reflectivity and reflectance anisotropy (RA) spectra of 5 silicon surfaces [(001), (113), (112), (111) and (110)] are calculated using the discrete dipole model. The structures used have bulk-terminated surfaces so that RA is found at the optical gap and above. A comparison is made between experimental RA spectra of H covered (001), (113) and (110) surfaces and the discrete dipole spectra and it is found that there is agreement for the (001) and (110) surfaces but the best fit to the experimental (113) surface spectrum is found for a (112) surface discrete dipole calculation. RA spectra are obtained using the McIntyre-Aspnes 3-layer model with surface layer and bulk dielectric functions taken from discrete dipole calculations. Surface excess dielectric functions are shown for these surfaces. It is found that, although RA spectra of the different surfaces are quite distinct, the gross features of the surface excess dielectric functions which are used to calculate them are quite similar. Thus small shifts in maxima and minima and differences in strength of these functions are responsible for the observed optical anisotropy, rather than distinct spectral features which differ from surface to surface. The surface dielectric function converges to the bulk value within 10 to 20 of the vacuum/solid interface, depending on frequency, so that RA at frequencies corresponding to the optical gap energy and above arises from this 20 region, rather than the topmost surface layer or layers.

(To appear i Phys. Rev. B)
Manuscripts available from: Charles.Patterson@tcd.ie

Spectral density of Samarium Sulphide

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Nöthnitzer Str. 38, 01187 Dresden, Germany
Manuel Richter and Helmut Eschrig
Institut für Theoretische Physik, Technische Universität,
01062 Dresden, Germany

Abstract

The spectral density of Samarium Sulphide is calculated using a multi-band periodic Anderson model. The s-, p- and d-states are treated as band states within the local density approximation. Realistic, local many-electron states of the $4f$-shell are taken into account. Using projection techniques a $4f$-occupation of 5.94 is found in the semiconducting phase. The calculated spectral density is in fair agreement with the measured photoemission and inverse photoemission spectra. To simulate the mixed-valent phase, the global hybridization strength between $4f$- and band states is empirically enhanced. The limits of a valence change controlled by the hybridization strength are discussed.

(Submitted to Phys. Rev. B)
Manuscripts available from: manuel@tmps16.mpg.tu-dresden.de

Low-field Hall coefficient of Al-4d dilute alloys: the role of the anisotropic impurity scattering

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Panepistimioupolis, GR-157 84 Zografos, Athens, Greece
G. Apostolopoulos, N. Boukos, and C. Papastaikoudis
Institute of Materials Science, National Centre for Scientific Research "Democritos"
GR-153 10 Aghia Paraskevi, Athens, Greece

Abstract

The role of the anisotropic impurity scattering in the determination of the low-field Hall coefficient of Al-4d dilute alloys is investigated by means of systematic theoretical calculations, as well as experimental measurements for Al-Zr and Al-Mo. The theoretical results, obtained without using any adjustable parameter, are in excellent agreement with the experimental data and a consistent interpretation of the systematic variation of the low-field Hall coefficient for aluminium-based dilute alloys with transition-metal impurities is given.

(Solid State Commun: in press)
Manuscripts available from: nstefan@atlas.uoa.gr

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

Susanne Handschuh and Stefan Blügel
Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

Abstract

We report systematic *ab initio* calculations for the magnetic moments, the magnetic coupling and the interlayer relaxation of the whole $3d$ transition–metal series (V, Cr, Mn, Fe, Co, Ni) as monolayers on the Fe(001) substrate. An energy analysis reveals that V and Cr prefer the layered antiferromagnetic coupling, Mn favors the $c(2\times2)$ ferrimagnetic superstructure and Fe, Co and Ni monolayers favor the ferromagnetic coupling to Fe(001). Cr and Mn on Fe exhibit a delicate interdependence of magnetism, film thickness and structure.

(Solid State Commun. **105**, 633 (1998).)
Latex-file available from: s.bluegel@kfa-juelich.de

Re-exchange controlled Diffusion in Surfactant-mediated Epitaxial Growth: Si on As-terminated Si(111)

K. Schroeder, B. Engels, P. Richard and S. Blügel
Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

Abstract

For a Si adatom on the Si(111) surface passivated by an As surfactant layer the adatom diffusion barrier (E_D), the exchange barrier (E_{EX}) for incorporation and the energy gain (E_B) due to incorporation into the As layer are calculated using an *ab initio* total energy and force method. We found that the activation energies for surface diffusion and exchange are similar in size and much smaller than the activation energy for the re-exchange (E_{REEX}) process ($E_D \sim E_{EX} << E_{REEX} = E_{EX} + E_B$). We propose that adatoms are rapidly incorporated into the As layer and the effective diffusion is determined by the re-exchange process.

(accepted at PRL)
Latex-file available from: schroed@iff138.iff.kfa-juelich.de

The Surface of Alloys – A New Magnetic Material

Ilja Turek
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Stefan Blügel
IFF, Forschungszentrum Jülich, D-52425 Jülich, Germany
Josef Kudrnovský
Institute of Physics, Academy of Sciences of the Czech Republic,
Na Slovance 2, CZ–18040 Praha, Czech Republic

Abstract

Based on *ab–initio* calculations we predict that the (100) surfaces of the RuV, RhV, and PdV binary alloys in the bcc structure are magnetic over a broad concentration range although they are nonmagnetic in the bulk and the metals V, Ru, Rh, and Pd are nonmagnetic in the bulk and at the surface. We find that the magnetic moment is basically located at the V site in the surface plane of the alloys and the V moment can be as large as about $1\mu_B$ for an alloy with 75% V concentration. The origin of the surface magnetism is traced back to a surface state of V(100), which becomes occupied due to alloying. Additional nonmagnetic alloys with magnetic surfaces are suggested.

(accepted in Phys. Rev. B Rapid Communications)
Latex-file available from: turek@ipm.cz

A Note on Origins and Implications of Orbital Ordering in $LaMnO_3$

I. V. Solovyev[1] and K. Terakura[2,3]
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1-1-4 Higashi, Tsukuba, Ibaraki 305-0046, Japan
JRCAT, National Institute for Advanced Interdisciplinary Research,
1-1-4 Higashi, Tsukuba, Ibaraki 305-8562, Japan
Institute of Industrial Science, University of Tokyo,
Roppongi, Minatoku, Tokyo 106, Japan

Abstract

Basic properties of the perovskite manganite $LaMnO_3$, the mother material of colossal-magnetoresistance manganites, are discussed based on the detailed band-structure calculations and also simple models. After giving some examples of success and failure of the band-structure calculations, detailed discussion is given on various features of the mutual relation among lattice distortion, electron correlation, orbital ordering and magnetic ordering. [Basically, the article contains results of model analysis for $LaMnO_3$, which were not included to our review article advertised in the previous newsletter because of the space limits.

(To be published in J. Korean Phys. Soc.: "Proceedings of Winter Workshop on Strongly Correlated Systems")
Manuscript available from: igor@jrcat.or.jp

Theoretical and experimental investigations on the magnetic EXAFS at the K- and $L_{2,3}$-edges of bcc-Fe

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Institut für Physikalische Chemie, Universität München,
Theresienstr. 37, D-80333 München, Germany
D. Ahlers and G. Schütz
Lehrstuhl für Experimentalphysik IV, Universität Würzburg,
Am Hubland, D-97074 Würzburg, Germany
L. Lemke, H. Wende, P. Srivastava and K. Baberschke
Inst. für Experimentalphysik, Freie Universität Berlin,
Arnimallee 14, D-14195 Berlin, Germany

Abstract

A fully relativistic theoretical description of magnetic EXAFS (MEXAFS) is presented that has been setup in the framework of relativistic multiple scattering theory on the basis of the Dirac equation for spin-polarised, magnetic solids. This approach is applied to supply a detailed interpretation of new and very accurate experimental data for the K- and $L_{2,3}$-edges of bcc-Fe that have been recorded for photon energies up to 600 eV above the Fermi level. In particular it is demonstrated that the MEXAFS spectra can be interpreted on the basis of the so-called sum rules.

(Accepted to Europhysics Letters)
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Electronic Structure of Cerium Monopnictides under Pressure

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Abstract

The electronic structures of the cerium monopnictides CeN, CeP, CeAs, CeSb and CeBi are calculated within the self-interaction corrected local-spin density approximation. This method allows for a description of the Ce f-electrons as either localized or delocalized, thus providing a unified scheme to describe the large volume ground states characterized by trivalent Ce ions as well as the low volume high pressure phases with tetravalent Ce ions. The structural phase transitions observed in CeP, CeAs, CeSb and CeBi are well described within this theory, as are the antiferromagnetic structures and semimetallic characteristics. The trends of the series may be understood in terms of the increasing localization of the f electron with increasing nuclear charge of the ligand.

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9 SCIENTIFIC HIGHLIGHT

Electrical conductivity of multilayer systems

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Abstract

Employing the Kubo-Greenwood formula the electrical conductivity of (disordered) layered systems is formulated in terms of the (Screened) Korringa-Kohn-Rostoker method and the Coherent Potential Approximation. In particular consequences with respect to bulk-like approaches and bulk-like concepts are pointed out. The present investigations are part of an intensive study of transport phenomena such as the Giant Magnetoresistance (GMR) and the Tunneling Magnetoresistance (TMR) in magnetic multilayers systems.

Introduction

A description of transport phenomena in multilayer systems requires conceptually new approaches that reflect the fact that such systems exhibit at best two-dimensional symmetry. However, in applying a new type of description, it is also mandatory to review typical bulk-like descriptions based on the use of three-dimensional translational symmetry, and to be able to recover results well-known from bulk studies. It is the aim of this contribution to show exactly these relations, but also to proof that the present numerical procedures are well-suited for theoretical studies of more complicated transport properties in multilayer systems such as the Giant Magnetoresistance or the Tunneling Magnetoresistance.

Theoretical description

General expressions

Suppose the electrical conductivity of a disordered system, namely $\sigma_{\mu\mu}$, is calculated using the Kubo-Greenwood formula (see [1], [2], [3], [4])

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{N_0\Omega_{at}} \left\langle \sum_{m,n} J^{\mu}_{mn} J^{\mu}_{nm} \delta(\epsilon_F - \epsilon_m)\delta(\epsilon_F - \epsilon_n) \right\rangle \quad . \tag{1}$$

In this equation $\mu \in \{x, y, z\}$, N_0 is the number of atoms, J^{μ} is a representation of the μ-th component of the current operator,

$$J^{\mu} = \{J^{\mu}_{nm}\} \quad ; \quad J^{\mu}_{nm} = \langle n \mid J_{\mu} \mid m \rangle \quad , \tag{2}$$

$\mid m\rangle$ is an eigenstate of a particular configuration of the random system, Ω_{at} is the atomic volume, and $\langle \cdots \rangle$ denotes an average over configurations. Eq. (1) can be reformulated in terms of the imaginary part of the (one-particle) Green's function

$$\sigma_{\mu\mu} = \frac{\hbar}{\pi N_0 \Omega_{at}} \mathrm{Tr} \ \langle J_{\mu} \mathrm{Im} G^{+}(\epsilon_F) J_{\mu} \mathrm{Im} G^{+}(\epsilon_F) \rangle \quad . \tag{3}$$

or by using "up-" and "down-" side limits, this equation can be rewritten [2] as

$$\sigma_{\mu\mu} = \frac{1}{4} \left\{ \widetilde{\sigma}_{\mu\mu}(\epsilon^{+}, \epsilon^{+}) + \widetilde{\sigma}_{\mu\mu}(\epsilon^{-}, \epsilon^{-}) - \ \widetilde{\sigma}_{\mu\mu}(\epsilon^{+}, \epsilon^{-}) - \widetilde{\sigma}_{\mu\mu}(\epsilon^{-}, \epsilon^{+}) \right\} \quad , \tag{4}$$

where

$$\epsilon^{+} = \epsilon_F + i\delta \quad , \quad \epsilon^{-} = \epsilon_F - i\delta \quad ; \quad \delta \to 0 \quad ,$$

and

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) = -\frac{\hbar}{\pi N_0 \Omega_{at}} \mathrm{tr} \ \langle J_{\mu} G(\epsilon_1) J_{\mu} G(\epsilon_2) \rangle \quad ; \quad \epsilon_i = \epsilon^{\pm} \quad ; \quad i = 1, 2 \quad . \tag{5}$$

The multiple scattering description

As in the bulk case [2], [3] for a layered system a typical contribution to the conductivity can be expressed [5] in terms of real space scattering path operators,

$$\begin{aligned} \widetilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) \quad = \quad & (C/N_0) \sum_{p=1}^{n} \sum_{i \in I(L_2)} \sum_{q=1}^{n} \\ & \left\{ \sum_{j \in I(L_2)} \mathrm{tr} \left\langle J^{pi}_{\mu}(\epsilon_2, \epsilon_1) \tau^{pi,qj}(\epsilon_1) J^{qj}_{\mu}(\epsilon_1, \epsilon_2) \tau^{qj,pi}(\epsilon_2) \right\rangle \right\} \quad , \end{aligned} \tag{6}$$

where $C = -\left(4m^2/\hbar^3 \pi \Omega_{at}\right)$ and $N_0 = nN$ is the total number of sites in the intermediate region (multilayer), as given in terms of the number of layers in the multilayer (n) and the order of the two-dimensional translational group N (number of atoms in one layer). In here and in the following the set of indices corresponding to the two-dimensional lattice L_2 is denoted by $I(L_2)$. Let $J^{p\alpha}_{\mu}(\epsilon_1, \epsilon_2)$ denote the angular momentum representation of the $\mu-$th component of the current operator according to component $\alpha = A, B$ in a particular layer p. Using a non-relativistic

formulation for the current operator, namely $\mathbf{J} = (e\hbar/im)\,\boldsymbol{\nabla}$, the elements of $J_\mu^{p\alpha}(\epsilon_1,\epsilon_2)$ are given by

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1,\epsilon_2) = \frac{e}{m}\frac{\hbar}{i}\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},\epsilon_1)^\dagger \frac{\partial}{\partial r_{p0,\mu}} Z^{p\alpha}_{\Lambda'}(\mathbf{r}_{p0},\epsilon_2) d^3r_{p0} \quad , \tag{7}$$

while within a relativistic formulation for the current operator, namely $\mathbf{J} = ec\boldsymbol{\alpha}$, one gets

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1,\epsilon_2) = ec\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},\epsilon_1)^\dagger \alpha_\mu Z^{p\alpha}_{\Lambda'}(\mathbf{r}_{p0},\epsilon_2) d^3r_{p0} \quad . \tag{8}$$

In Eqs. (7), (8) the functions $Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},z)$ are scattering solutions [3] and WS denotes the volume of the Wigner-Seitz sphere. It should be noted that

$$J^{p\alpha}_{\mu}(\epsilon_1,\epsilon_2) = J^{p0,\alpha}_{\mu}(\epsilon_1,\epsilon_2) = J^{pi,\alpha}_{\mu}(\epsilon_1,\epsilon_2) \quad , \quad \forall i \in I(L_2) \quad . \tag{9}$$

¿From the brackets in Eq. (6), one easily can see that for each layer p the first sum over L_2 yields N times the same contribution, provided two-dimensional invariance applies in all layers under consideration. Assuming this kind of symmetry (see Sec. II), a typical contribution $\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2)$ to the conductivity is therefore given by

$$\begin{aligned}\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) \;&=\; (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n} \\ &\left\{\sum_{j\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad ,\end{aligned} \tag{10}$$

where $p0$ specifies the origin of L_2 for the p-th layer. Just as in the bulk case [2], [3] this kind of contribution can be split up into a (site-) diagonal and a (site-) off-diagonal part,

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \widetilde{\sigma}^0_{\mu\mu}(\epsilon_1,\epsilon_2) + \widetilde{\sigma}^1_{\mu\mu}(\epsilon_1,\epsilon_2) \quad . \tag{11}$$

Site-diagonal conductivity

By employing the CPA condition discussed in full detail in Ref. [5] and omitting vertex corrections, for the diagonal part ($p0 = qj$) one simply gets,

$$\begin{aligned}&\widetilde{\sigma}^0_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/n)\sum_{p=1}^{n}\sum_{\alpha=A,B} c^\alpha_p \mathrm{tr}\left[\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_{c}(\epsilon_1)J^{p\alpha}_{\mu}(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_{c}(\epsilon_2)\right] \quad ,\end{aligned} \tag{12}$$

where

$$\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1) = \widehat{D}^{pp}_{\alpha}(\epsilon_2)^t J^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\widehat{D}^{pp}_{\alpha}(\epsilon_1) \quad . \tag{13}$$

Site-off-diagonal conductivity

The off-diagonal part can be partitioned into two terms

$$\widetilde{\sigma}^1_{\mu\mu}(\epsilon_1,\epsilon_2) = \widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) + \widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) \quad , \tag{14}$$

where

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq}) \left\{\sum_{j\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad , \tag{15}$$

and

$$\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n}\delta_{pq} \left\{\sum_{(j\neq 0)\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad . \tag{16}$$

As one can see $\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2)$ arises from pairs of sites located in *different* layers, whereas $\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2)$ corresponds to pairs of sites in *one and the same* layer (excluding the site-diagonal pair already being accounted for in $\widetilde{\sigma}^0_{\mu\mu}(\epsilon_1,\epsilon_2)$). In general the averaging of $\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2)$ is given by

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \times \mathrm{tr}\left\{J^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\left\langle\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle_{p0\alpha,qj\beta}\right\} \quad . \tag{17}$$

By employing the CPA condition and omitting vertex corrections (see Ref. [5]), $\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2)$ is found to reduce to

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \times \mathrm{tr}\left\{\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}_{c}(\epsilon_1)\widetilde{J}^{q\beta}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}_{c}(\epsilon_2)\right\} \quad . \tag{18}$$

Since the site-off-diagonal scattering path operators $\tau^{p0,qj}_{c}(z)$ are defined as

$$\tau^{p0,qj}_{c}(z) = \Omega^{-1}_{SBZ}\int e^{i\mathbf{k}\cdot\mathbf{R}_j}\hat{\tau}^{pq}(\mathbf{k},z)d^2k \quad , \tag{19}$$

in a manner similar as in the bulk case the orthogonality for irreducible representations of the two-dimensional translation group can be used:

$$\sum_{j\in I(L_2)}\tau^{p0,qj}_{c}(\epsilon_1)\tau^{qj,p0}_{c}(\epsilon_2) = \Omega^{-1}_{SBZ}\int\hat{\tau}^{pq}(\mathbf{k},\epsilon_1)\hat{\tau}^{qp}(\mathbf{k},\epsilon_2)d^2k \quad , \tag{20}$$

For $\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2)$ one therefore gets the following expression

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\,\Omega^{-1}_{SBZ}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \mathrm{tr}\int\left\{\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\hat{\tau}^{pq}_{c}(\mathbf{k},\epsilon_1)\widetilde{J}^{q\beta}_{\mu}(\epsilon_1,\epsilon_2)\hat{\tau}^{qp}_{c}(\mathbf{k},\epsilon_2)d^2k\right\} \quad . \tag{21}$$

The last term in Eq. (14) to be evaluated is $\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2)$ corresponding to the case that two sites are located in one and the same layer,

$$\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\Omega^{-1}_{SBZ}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{p} \mathrm{tr}\int\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\hat{\tau}^{pp}_{c}(\mathbf{k},\epsilon_1)\widetilde{J}^{p\beta}_{\mu}(\epsilon_1,\epsilon_2)\hat{\tau}^{pp}_{c}(\mathbf{k},\epsilon_2)d^2k\right\} + \widetilde{\sigma}^{3,corr}_{\mu\mu}(\epsilon_1,\epsilon_2) \quad , \tag{22}$$

where $\widetilde{\sigma}_{\mu\mu}^{3,corr}(\epsilon_1,\epsilon_2)$ arises from extending the sum to $\forall j \in I(L_2)$ and subtracting a corresponding correction term of the form

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}^{3,corr}(\epsilon_1,\epsilon_2) = \\ &= -(C/n)\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right] \quad .\end{aligned} \tag{23}$$

Total conductivity for layered systems

Combining now all terms, a typical contribution $\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2)$ to the conductivity is given by

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/n)\sum_{p=1}^{n}\left\{\sum_{\alpha=A,B} c_p^\alpha \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)J_\mu^{p\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right. \\ &- \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right] \\ &\left.+ \Omega_{SBZ}^{-1}\sum_{q=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\int\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pq}(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{q\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{qp}(\mathbf{k},\epsilon_2)d^2k\right]\right\} \quad .\end{aligned} \tag{24}$$

Comparing the last equation with the corresponding bulk result [2],

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/\Omega)\left\{\sum_{\alpha=A,B} c^\alpha \mathrm{tr}\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\epsilon_1)J_\mu^{\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\epsilon_2)\right]\right. \\ &- \sum_{\alpha,\beta=A,B} c^\alpha c^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\epsilon_1)\widetilde{J}_\mu^{\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\epsilon_2)\right] \\ &\left.+ \Omega_{BZ}^{-1}\sum_{\alpha,\beta=A,B} c^\alpha c^\beta \mathrm{tr}\int\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\mathbf{k},\epsilon_2)d^3k\right]\right\} \quad ,\end{aligned} \tag{25}$$

where Ω is the volume of the unit cell, one easily can see that in both cases one has the same "formal structure", however, for layered systems a summation over layers occurs for the diagonal term and a double sum over layers for the off-diagonal term, which is a direct consequence of the fact that in the growth direction of multilayers no translational invariance applies.

Defining finally layer-diagonal terms as

$$\begin{aligned}\widetilde{\sigma}_{\mu\mu}^{pp}(\epsilon_1,\epsilon_2) = \quad &(C/n)\sum_{\alpha=A,B} c_p^\alpha\left\{\mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)J_\mu^{p\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right. \\ &\left.- \sum_{\beta=A,B} c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right\} \quad ,\end{aligned} \tag{26}$$

and layer-off-diagonal terms as

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1,\epsilon_2) = (C/n\Omega_{SBZ}) \\ &\quad\times\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\left[\int \widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pq}(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{q\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{qp}(\mathbf{k},\epsilon_2)d^2k\right] \quad ,\end{aligned} \tag{27}$$

$\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2)$ can be written as

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \sum_{p=1}^{n}\left\{\widetilde{\sigma}_{\mu\mu}^{pp}(\epsilon_1,\epsilon_2) + \sum_{q=1}^{n}\widetilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1,\epsilon_2)\right\} \quad . \tag{28}$$

Numerical applications

All calculations reported here are based on the fully relativistic spin-polarized Screened KKR method for generating the corresponding selfconsistent scattering potentials as well as for the evaluation of the electric conductivity tensor. In the former case a total of 45 $\mathbf{k}_{||}$ points in the irreducible wedge of the surface Brillouin zone is used, for the latter 1830 $\mathbf{k}_{||}$ points. The following systems were investigated as precursor cases for a study of the giant magnetoresistance in Co/Cu multilayers

Substrate	Cu(100)
Multilayer	$(\mathrm{Cu})_n \quad , n = 1, 45$
Cap	Cu(100)

Substrate	Cu(100)
Multilayer	$(\mathrm{Co})_n \quad , n = 1, 39$
Cap	Cu(100)

Substrate	Cu(100)
Multilayer	$(\mathrm{Cu}_{0.85}\mathrm{Co}_{0.15})_n \quad , n = 1, 30$
Cap	Cu(100)

As is well-known from bulk theory, (at zero temperature) for fcc Cu the resistance is exactly zero, whereby for the tensor elements the relation

$$\rho_{xx} = \rho_{yy} = \rho_{zz}$$

applies. Quite clearly by using Eq. (28) this will only be the case if the number of layers to be summed over is sufficiently large, a fact, which of course supplies an excellent test of the applied numerical means.

In Figure 1 the resistivities $\rho_{xx}(= \rho_{yy})$ and ρ_{zz} ($\rho_{\mu\mu} = 1/\sigma_{\mu\mu}$) are shown as a function of the number of layers of Cu on top of a Cu(100) substrate and capped semi-infinitely by Cu(100). Since $n\rho_{\mu\mu}$ shows a linear behavior with respect to n (for sufficiently large n) the curves can be extrapolated to very large n. As one can see in this Figure ρ_{xx} and ρ_{zz} indeed go exactly to zero as in Eq. (28) the number of layers increases. In addition, for a large enough number of layers one loosely could state that cubic symmetry is "restored".

In order to understand this Figure and also the following ones properly, it is necessary to recall that this reflects nothing but the fact that as compared to the bulk expression Eq. (25) in Eq. (28) the "missing" lattice Fourier transformation in one direction, namely in direction of the surface normal, shows up as a finite sum. In principle, therefore, only as n approaches the order of the translational group for translations along the surface normal, a bulk-like result can be expected. This has important consequences for realistic multilayer systems, in which the number of layers can be rather small: "confinement" effects apply in such systems and even for a system with growth direction (100) in general

$$\rho_{xx} \neq \rho_{zz} \quad .$$

It is very reassuring that the numerical procedures applied indeed show the correct behavior discussed above (as n becomes very large).

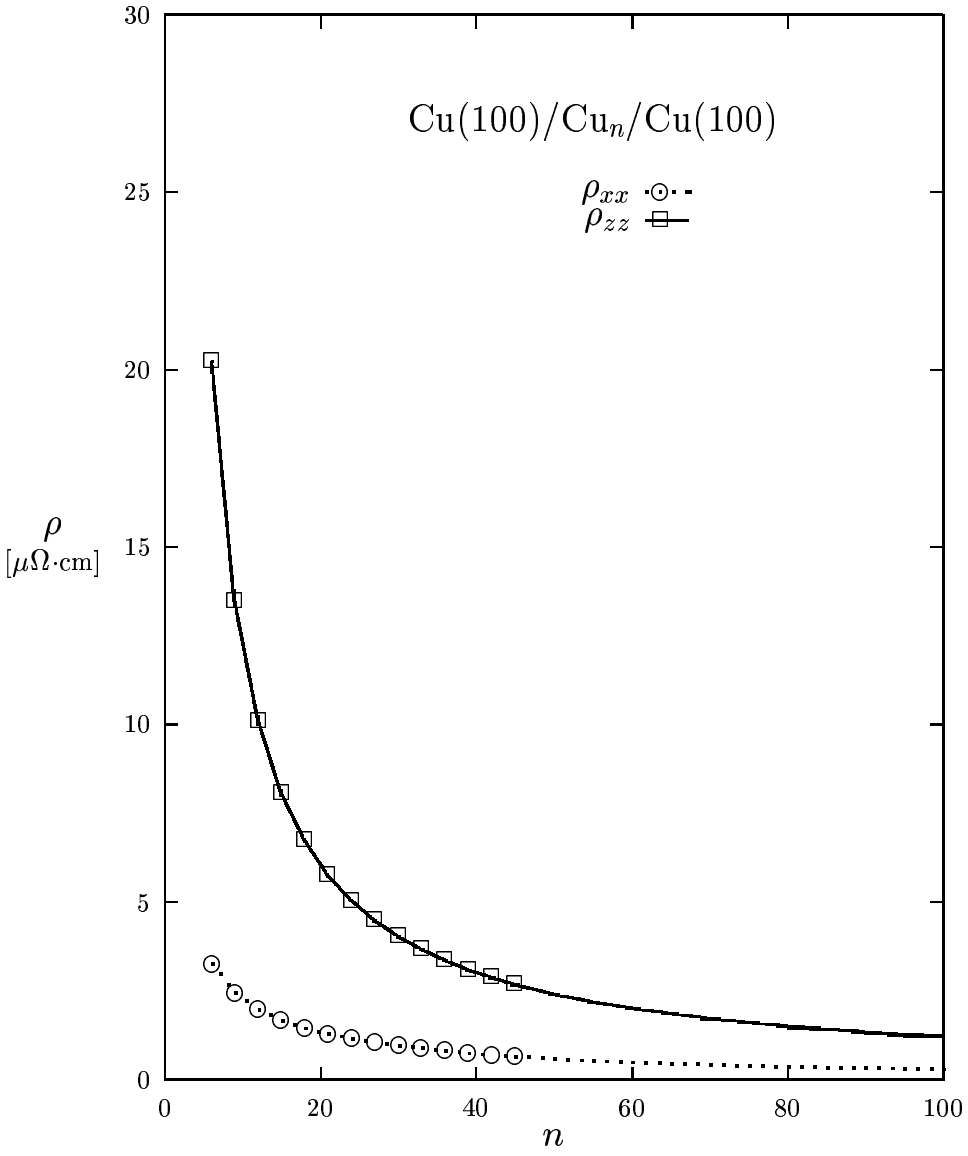

Figure 1: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/Cu$_n$/Cu(100) as a function of the number of Cu-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

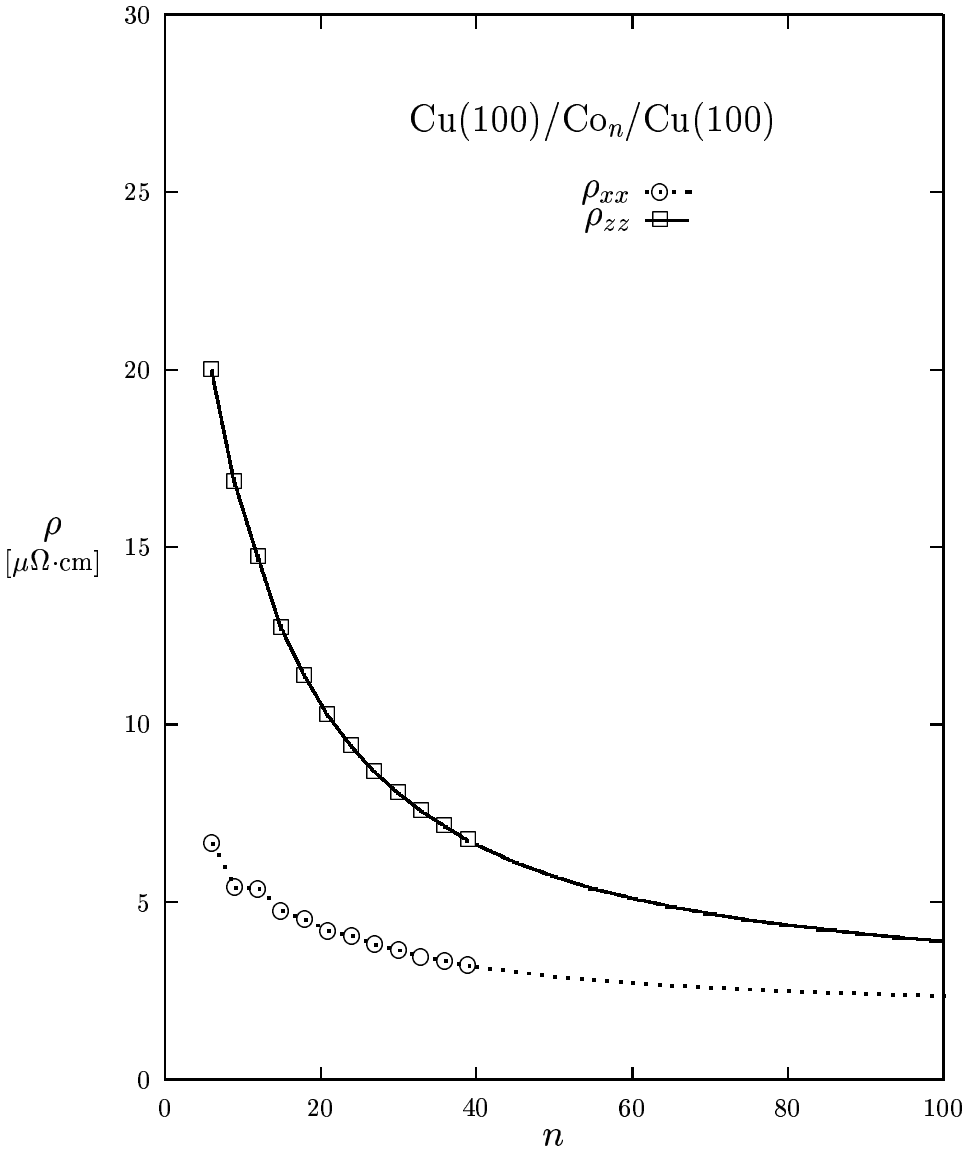

Figure 2: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/Co$_n$/Cu(100) as a function of the number of Co-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

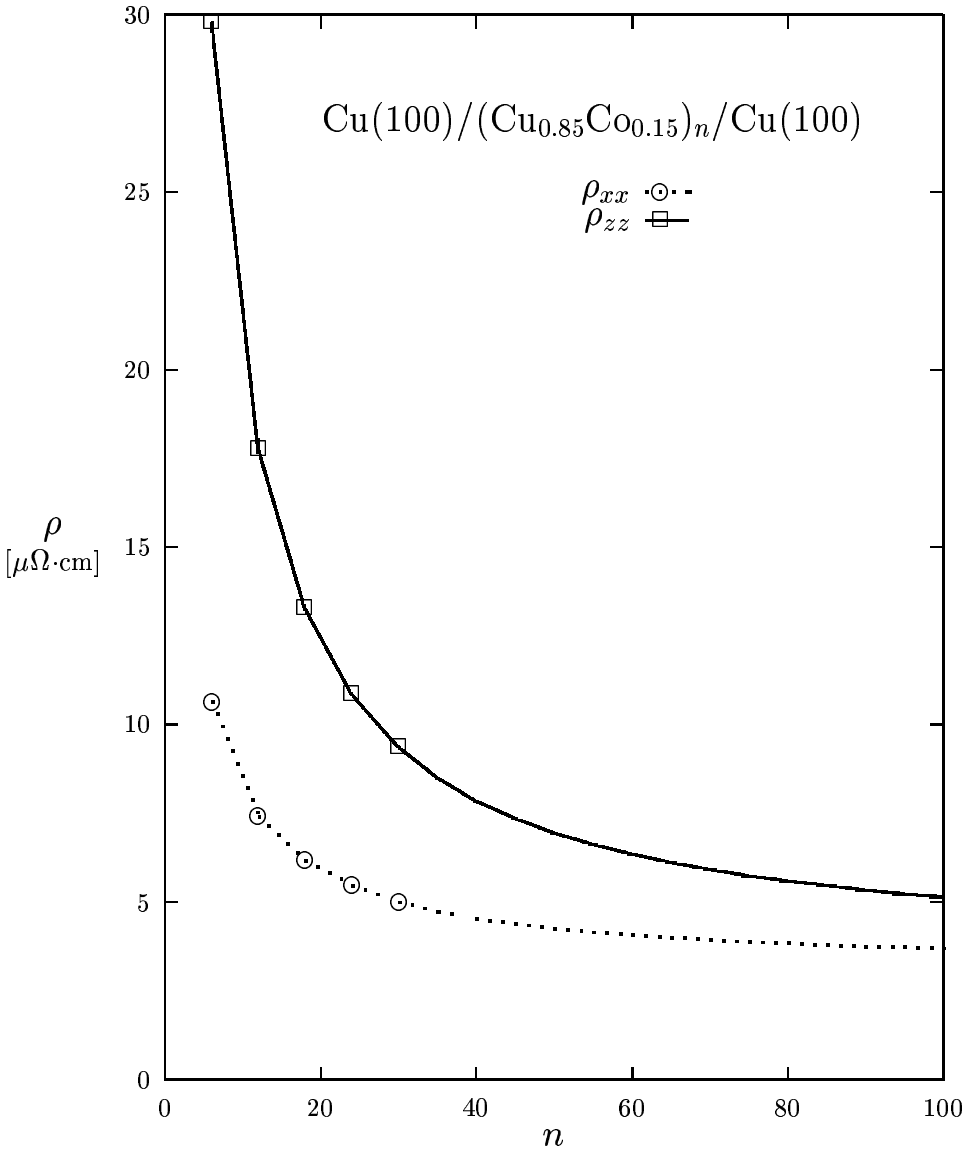

Figure 3: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/$(Cu_{0.85}Co_{0.15})_n$/Cu(100) as a function of the number of $(Cu_{0.85}Co_{0.15})$-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

In Figures 2 and 3 the same type of display is shown when the multilayer consists of a finite number of Co-layers and a finite number of statistically disordered ($Cu_{0.85}Co_{0.15}$) layers, respectively. In these two cases as the number of layers increases the resistivities cannot approach zero, but have to tend to a constant. As one can see this is indeed the case. In the case of pure Co layers one could call this constant a "contact" contribution to the resistivity. For the alloy case it is interesting to observe, that for large enough n the resistivity is of the same order of magnitude that characterizes the resistivity of noble metal rich alloys with transition metals. Of course the constant obtained and to be seen in Figure 3 is not quite the resistivity for a bulk alloy of fcc $Cu_{0.85}Co_{0.15}$ since (a) the lattice constant and the Fermi energy of pure Cu apply and (b) the meaning of a "contact" resistivity pertains. Only in the case that the (semi-infinite) substrate and the (semi-infinite) cap are of the same material – $Cu_{0.85}Co_{0.15}$ in the present example – the resistivity for large enough n picks up the meaning of a residual resistivity. It should be noted that even though the present examples are meant to serve as numerical tests, it is evident that such systems very well can serve as example for an ab-initio calculation of "contact" resistivities which otherwise are computationally inaccessible.

Presently the method and numerical techniques illustrated in this contribution are applied to a study of the giant magnetoresistance (GMR) in Co/Cu multilayer systems and also for studying the effect of repetitions ("repeats") of multilayers as is the case in most experimental systems on the GMR.

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