Ψ_k Newsletter

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

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Contents

1 Editorial

In this Newsletter in the TMR1 section there is a report on the Mini-Workshop on *'Tunnelling Magnetoresistance'*. In the TMR2 section we have an announcement of the FP-LAPW Workshop, which is already the sixth in its series. The workshop is traditionally set in Vienna and is supported by both the TMR2 Network and the ESF Programme. In the **ESF Programme** section we have announcements of future workshops supported by this programme, and a report on the Madrid Mini-Workshop. In that section there are also reports on collaborative visits. In the **UK's CCP9 Programme** section there is a report on the workshop dedicated to *'Mesoscopic Superconductors and Hybrid Systems'*. The reports in both the **ESF** and **CCP9** sections contain a large number of abstracts of talks presented at those workshops. Additionally, as always, there are a few abstracts in the usual **Abstracts** section. Announcements of available positions can be found in the **General Job Announcements** section. Announcements of meetings/workshops are in the **General Workshop/Conference Announcements** section. In this newsletter we also have a small section presenting other initiatives in our field. This section is called **Presenting Other Initiatives**, and there Rex Godby (*University of York*) writes about an RT 'NANOPHASE' Network on "*Nanoscale photon absorption and spectroscopy with electrons*". The scientific highlight is by A. Svane (*University of Aarhus, Denmark*) *et al.* on **"Self-Interaction Corrected Electronic Structure of Rare Earths"**.

Please check the table of contents for further details.

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

http://psi-k.dl.ac.uk/

The above contains pointers to home pages of some of the members of our electronic structure community. 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 note that the home page of the Psi-k Networks has recently been updated. It contains useful information regarding funding of workshops and collaborative visits within the ESF Programme. Its major new feature is a separate highlight section which contains all highlight articles of the Newsletters published so far.

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
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2 General News

2.1 Psi-k 2000 Conference

Schwäbisch Gmünd, 22-26 August, 2000

”Ab Initio (from Electronic Structure) Calculations of Complex Proceses in Materials”

First a big thank you to everyone for submitting about 500 names for possible invited speakers for the conference. It has been a wonderful flood and display of impressive research. It is good that we had set up an unusualy large Programme Committee for selecting among them, so that knowledge about work from all across Europe and to some extent the rest of the world was covered, as were all areas of research. The list of invited speakers will soon be posted on the conference web site:

http://psi-k.dl.ac.uk/psi-k2000

At the above page you will also be able to find out when to submit abstracts, register to the conference and book a hotel in Schwaebisch Gmuend. The ACCOMODATION bureau and the conference REGISTRATION (with fee!)will both open some time in April, both strictly on the basis of first-come-first-served: please watch the conference web site given above.

We look forward to seeing you there.

Paul Durham, Psi-k2000 Conference Chairman
Volker Heine, Chairman, ESF Psi-k Programme

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Reports on Workshops

3.1.1 Report on Miniworkshop

"Tunnelling Magnetoresistance"

A TMR-Miniworkshop on "Tunnelling Magnetoresistance" took place on January 13-14, 2000 at the University Paris-Sud/Orsay. It was attended by the following persons:

Charles Sommer, CNRS-Orsay

Peter H. Dederichs, Phivos Mavropoulos, Nikolaos Papanikolaou (all of Research Center Jülich)

Albert Fert, Jose M. de Teresa, Dante Mosca, Frederic Petroff, Vincent Cros (all of UMR CNRS-Thomson, Orsay)

Peter M. Levy (New York University, USA)

The aim of the workshop was to review the current activities on tunnelling in the different groups and to identify interesting problems for future research and collaborations. In total five talks were given on Friday afternoon and the Saturday morning was used for intensive discussions. The titles of the talks are:

N.Papanikolaou	*STM Spectra of Transition Metal Impurities on the Fe(001) Surface*
Ph. Mavropoulos	*Complex Bandstructure and Tunnelling through Ferromagnet/Insulator/Ferromagnet Junctions*
F.M. de Teresa	*Spin Polarization of Co in Magnetic Tunnel Junctions*
D. Mosca	*Spin Polarized Transport in Fe/ZnSe/Fe Heterostructures*
P.M. Levy	*Contributions from Interface States to Tunnelling Conductance*

The groups of Albert Fert and Peter Levy will be our partners in the future RT-Network on "Computational Magnetoelectronics".

Thanks to Chuck Sommers for the local organisation.

Peter H. Dederichs

4 News from the TMR2 Network

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

4.1 Workshop Announcements

4.1.1 FPLAPW Workshop

Sixth WIEN Workshop

Full-Potential LAPW calculations with the WIEN97 code

April 26-29, 2000
Vienna University of Technology, Austria
Chairman: Karlheinz Schwarz (TU-Vienna)
Email: kschwarz@theochem.tuwien.ac.at

Supported by TMR2 (LAPW) and ESF Program STRUC-Ψ_k.

First Announcement

This workshop (within the Psik network) is concerned with recent progress in density functional calculations using the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the WIEN97 code (or related topics).

The workshop will be organized (in two parts) as follows:

- Part I:
  - A short introduction to the LAPW method and the density functional theory
  - Introduction to the use of the WIEN97 program package
  - Hands-on experience
- Part II:
  - Results obtained with LAPW (WIEN97) and related topics
  - Discussion and exchange of experience
  - Poster session

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

Contact:
For further information look at our WWW-homepage
http://www.tuwien.ac.at/theochem/wien97/ws2000/
or send an email to kschwarz@theochem.tuwien.ac.at.

5 News from the ESF Programme

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

5.1 Future Workshops

At its meeting in October 1999, the core steering group of the ESF funded part of the Psi-k Network approved funding for the following 10 workshops and hands-on course in 2000.

1. Workshop on "Catalysis from First Principles" to be held in Berlin on 5-8 July 2000 and organised by J. Hafner, J. Norskov and M. Scheffler. This workshop would be a follow-up of the industry workshop held in 1998 and the Catalysis workshop held in Denmark in May 1999.

2. Workshop on "Computational Materials Science 2000", to take place in Sardinia on 8-11 September 2000 and organised by V. Fiorentini, P. Ruggerone, F. Meloni and A. Baldereschi.

3. "Across the Length Scales II: Applications (MML2000)". This workshop, organised by D.G. Pettifor, A.P. Sutton, R.E. Rudd, S.D. Kenny would take place in Oxford in July 2000. It would focus on the use of multiscale modelling to describe the processing of materials.

4. Workshop on "Excited States and Electronic Spectra" to take place in CECAM, Lyon in July 2000 and organised by L. Reining, G. Onida and A. Rubio.

5. Workshop on "Advances in First-Principles Computational Condensed Matter Physics" to be held in Madrid on 13-15 January 2000 and organised by E. Artacho, A. Garcia and P. Ordejon. Every second year the ICTP in Trieste organises an important workshop on Total Energies and Forces Methods. Every other year a mini-workshop takes place, partly to plan the next conference.

6. Workshop on "Electronic and Optical Properties of Semiconducting Glasses" to be held in CECAM (Lyon) in May-June 2000 and organised by D. Drabold, G. Barkema, N. Mousseau and P. Ordejon.

7. Workshop on "Future Developments in the study of structure-property relations by computational crystallography and experiments" to be held at CECAM in late 2000 and organised by B. Winkler and V.Millman. This proposed workshop is planned to provide an opportunity to discuss the state of the art of crystallographic, crystal chemical and physical investigations of inorganic compounds and to bring together experimentalists and code-developers with different backgrounds.

8. "Extended Defects in Semiconductors" to be held at the University of Sussex on 18-22 July 2000 and organised by M. Heggie. This conference follows on from EDS 98 held at Jaszowiec, Poland and EDS 96 in Hyères, France.
9. The Vth European Workshop on Solving the Bogoliubov de Gennes Equations, organised by B.L. Gyorffy and E.K.U. Gross, to take place on April 14-16, 2000 at Bristol University. This workshop is co-organised by TMR2 and CCP9.
10. Hands-on LAPW Course to be organised by S. Bluegel.

Further information on these workshops will be published on the homepage of the psi-k network (http://psi-k.dl.ac.uk).

5.2 Workshop Announcements

5.2.1 CECAM - ESF/Psi-k Workshop

Future developments in the study of structure-property relations by 'computational crystallography' and experiments

CECAM - ESF/Psi-k

Lyon, France

23-27/10/2000

In the autumn of 2000 we will hold a workshop on "Future developments in the study of structure-property relations by 'computational crystallography' and experiments" at CECAM in Lyon, France. This workshop will be similar in duration and number of participants to our last workshops:

`http://www.min.uni-kiel.de/kristallographie/cecam97/seite_01.html`
`http://www.min.uni-kiel.de/kristallographie/esf/`

The emphasis this time will be on recent experimental and theoretical developments in the spectroscopic investigation of solids, such as vibrational-, core-level-, nmr-, and optical-spectroscopy. Contributions on recent results on defect studies, surfaces, electron densities, compression mechanisms of structures and so on are, however, also welcome.

The main point, as in the earlier meetings, is to discuss the state-of-the-art of the available theoretical approaches and current experiments and, at the same time, to think about future developments.

There will be some financial support for participants by CECAM and the ESF/Psi-k. We are now beginning to finalise the program and the number of participants will be limited to about 25.

If you'd like to participate, please send us the title of your planned contribution to any of the organising committee . All participants should plan to submit an extended abstract of about 5 pages by the end of August.

We have begun to set up a web-page at:

http://www.min.uni-kiel.de/kristallographie/cecam2000/

where we will post any further information.

We look forward very much to hearing from you.

The organising committee:

Bjoern Winkler (bjoern@min.uni-kiel.de)
Victor Milman (vmilman@msicam.co.uk)
Karsten Knorr (knorr@min.uni-kiel.de)
Chris Pickard (cp@min.uni-kiel.de)

5.3 Reports on Workshops

5.3.1 Report on Madrid Mini-Workshop

WORKSHOP "ADVANCES IN FIRST-PRINCIPLES COMPUTATIONAL CONDENSED MATTER PHYSICS"

Sponsored by	The European Science Foundation Programme STRUC-Ψ_k
	Universidad Autónoma de Madrid
	Universidad del País Vasco
	Spanish Consejo Superior de Investigaciones Científicas
	Motorola PSRL and FPD
Organised by	Emilio Artacho, Universidad Autónoma de Madrid (Spain)
	Alberto García, Universdad del País Vasco (Spain)
	Pablo Ordejón, ICMAB-CSIC (Spain)
Scientific Committee	A. Baldereschi, EPFL, Laussanne (Switzerland)
	S. Baroni, SISSA, Trieste (Italy)
	M. Gillan, University College of London, London (UK)
	K. Kunc, CNRS, University P. and M. Curie, Paris (France)
	S. Louie, University of California - Berkeley (USA)
	R. M. Martin, University of Illinois at Urbana-Champaign (USA)
	M. Methfessel, Inst. für Semicond. Physics, Frankfurt-Oder (Germany)
	R. Needs, Cambridge University, Cambridge (UK)
	M. Parrinello, MPI-FKF, Stuttgart (Germany)
	K. Terakura, NAIR, Tsukuba (Japan)
	D. Vanderbilt, Rutgers University, Rutgers (USA)
	E. Wimmer, Molecular Design s.a.r.l., Le Mans (France)

This meeting is related to the series held regularly (in January in odd-numbered years) at the Abdus Salam International Center for Theoretical Physics in Trieste (Italy). These rather large ("MAXI") workshops were originally labeled as dealing with "Total Energies and Forces Methods", and currently with "Electronic Structure Theory and Simulations". In even-numbered years, a smaller ("MINI") workshop is held at different venues. The last MINI was held in Tsukuba, in January 1998. Following the tradition of the previous MINI's, the Madrid workshop was devoted to recent advances in computational condensed matter physics, based on realistic calculations of the electronic structure of polyatomic systems.

The workshop took place in “La Cristalera”, a conference center owned and maintained by the Universidad Autonoma de Madrid, and located in Miraflores, about 40 km north of the city. Transportation to and from the conference center was arranged by the organization. The center provided a quiet environment, with meals and accommodation at the same building, which facilitated discussion and contact.

The workshop was an eventful one. The heaviest snowfall in fifteen years caused a power outage in the Northwest of Madrid province that affected the workshop venue. This forced the relocation of the attendees and a delay of several hours of the start of the Friday session. The program was completed (except for two talks) by tightening the schedule.

The format consisted in 19 invited talks of 40 minutes plus 10 minutes of discussion (after the relocation, the time allocated for talks was reduced to 25+5 minutes). Besides the invited talks, there was a display of contributed posters. (There was no specific poster session, but there was time for discussion in between and after the talks.) While waiting (vainly) for the power to be restored, a round table was organized. Among the issues raised were the pros and cons of the use of ab-initio program packages and the possibility of building a public-access repository of routines. It was agreed to work on the idea and make it concrete at the next Trieste meeting, in January 2001.

The workshop was organized around four main topics:

1. Density-functional Molecular Dynamics and Monte Carlo

   Mike Gillan gave a review of the recent work on the calculation of free energies of solids and liquids, aimed at the determination of the melting curves of solids, and the new developments to calculate chemical potentials in solutions. He also described the application to the physics of the inner Earth’s core. **Rafael Ramirez** was invited to talk about the recent developments in using Path Integral Monte Carlo simulations to obtain dynamical properties and excitation energies of quantum systems. However, his talk was one of the two that were canceled due to the power problems. **Richard Needs** described methods to calculate excited electronic states by means of fixed-node diffusion quantum Monte Carlo. He discussed problems associated with these calculations, in particular the lack of a variational principle of general validity for the excitation energies.

2. Theory of magnetic and electronic polarization

   Ivo Souza gave a talk about the relation between electronic localization and polarization in insulators. Using a generating function approach he showed how these quantities are intimately related, and gave nice connections to the well known Kohn’s theory of the insulating state, in terms of the decomposition of the many-body wave function in localized (disconnected) wave functions. **Stefano Baroni** described a method to study the spin dynamics in ferromagnetic systems, by means of an adiabatic decoupling of the spin and charge excitations. The method provides an excellent description of the magnon spectrum of iron, and should be much more efficient than other current linear response methods (although it cannot describe Stoner-type excitations). **Warren Pickett** talked about the recently discovered coexistence of ferromagnetism with singlet superconductivity in ruthenocuprates. He argued about the origin of this coexistence, in terms of the spatial separation of the orbitals responsible for the magnetism (Ru t_{2g}) and for the superconductivity (Cu $d_{x^2-y^2}$).

3. Time Dependent DFT

   Xavier Gonze discussed on the conceptual aspects of TD-DFT, concerning the formalism (and its connection to many-body perturbation theory), and the use of different potentials and kernels. He showed results for the excited states potential energy surface of $(HeH)^+$, and showed that, comparing to CI results, the exchange-only Optimized Effective Potential performs considerably better then the LDA one. **Kazuhiro Yabana** presented a method to calculate the optical response of finite systems, by integration of the the time-dependent Kohn-Sham equations in real-time and space. The quadratic scaling of the method with the size of the system allows its use in considerably large systems, with a few hundreds of electrons. **Kieron Burke** also discussed about the basic approximations of TD-DFT and their accuracy, and on the performance of different XC kernels.

4. Applications

   Several applications of first principles calculations were presented in the workshop. An important number of them corresponded to materials related problems, but other fields were also covered.

   With regards to materials, several talks were delivered. **Erich Wimmer** gave a presentation on the combination of electronic structure methods with large-scale database analysis to understand and predict the properties of materials, and presented some commercial tools in this direction. **Chris van de Walle** presented calculations of defect and impurity states in III-nitride semiconductors. He addressed the issue of the limitations of DFT for these calculations, and showed how these can be overcome with the use of self-interaction and relaxation-corrected pseudopotentials (although the ability of computing the total energy is lost). **Magdalena Siodmiak** discussed schemes to tackle the complex problem of CVD growth, with the aid of first principles total energy calculations. **Nathalie Vast** showed calculations of the structure and vibrational properties of icosahedral B_4C, and detailed comparison with experimental data. **David Singh** presented a talk on the use of DFT calculations in the search for new thermoelectric materials. He described the properties which a good thermoelectric material should have, and ideas on how to engineer materials with these properties. The main problem is that these properties (mainly, low thermal conductivity and high electrical conductivity) are to a large extent contradictory. He showed how first principles theory can help in optimize the performance of designed materials. **Ruben Perez** was invited to talk about tip-surface interactions on semiconductor surfaces, but his talk was canceled.

   There were also several talks on applications to problems other than those of traditional materials science. **Jose M. Soler** and **Daniel Sanchez-Portal** talked about the recent applications of order-N LCAO DFT calculations to several complex systems: DNA, liquid silicon surfaces, zintl manganites and monoatomic gold wires. **Carme Rovira** presented her work on the modelization of biological molecules, and in particular, in HEME systems. She showed results on the ligand binding properties of myoglobin, with special emphasis on the different behavior of several ligands (O_2, CO and NO). **Björn Winkler** discussed the usefulness of first principles DFT calculations in Mineralogy and Crystallography, in particular in the prediction of pressure and temperature-induced structural changes of minerals.

PROGRAM

THURSDAY 13

9:30 Conference Opening (E. Artacho)

9:50 Erich Wimmer (Materials Design s.a.r.l., France)
Combination of Electronic Structure Methods and Large-scale Data Analysis: A Tool for Understanding and Innovation

10:40 — Coffee —

11:20 Ivo Souza (University of Illinois, USA)
Polarization and Localization in Insulators: Generating Function Approach

12:10 Richard Needs (Cambridge, UK)
Fixed-node diffusion quantum Monte Carlo calculations of excited states

13:00 — Lunch —

15:00 Chris Van de Walle (Xerox, Palo Alto, USA)
First-principles calculations of defects and impurities in GaN, AlN, and InN

15:50 Magdalena Siodmiak (Marburg, Germany)
Gas Phase Reactions in Chemical Vapor Deposition of Transition Metal Compounds

16:40 — Coffee —

17:10 Nathalie Vast (CEA, France)
The atomic structure and vibrational properties of icosahedral B_4C *boron carbide*

18:00 David Singh (NRL, USA)
Using Density Functional Calculations to Find New Thermoelectric Materials

FRIDAY 14

11:00 Round Table

16:00 — Relocation of Workshop —

19:00 Carme Rovira (Universitat de Barcelona, Spain)
Modeling the ligand binding properties of myoglobin by first-principles molecular dynamics

19:30 Xavier Gonze (Louvain, Belgium)
—it Excitation energies from Density Functional Theory

20:00 Jose M. Soler (Harvard University, USA)
Siesta *applications: from biomolecules to liquid surfaces*

20:25 Daniel Sánchez-Portal (University of Illinois, USA)
Applications of Siesta *to metallic systems: gold monatomic wires and zintl manganites*

20:50 — Dinner —

22:15 Warren Pickett (U. C. Davis, USA)
Magnetoelectronic Character of a Superconducting Cuprate

22:45 Stefano Baroni (SISSA, Italy)
Magnons in real materials from density-functional theory

SATURDAY 15

9:00 Kazuhiro Yabana (Tsukuba University, Japan)
Real-time method for optical response of clusters and molecules
9:30 Kieron Burke (Rutgers University, USA)
Developement of time-dependent density functional theory
10:00 Mike Gillan (University College of London, UK)
Ab-initio free energies and the composition of the Earth's core
10:30 — Coffee —
11:00 Björn Winkler (University of Kiel, Germany)
Recent Advances in Computational Crystallography / Mineralogy
11:30 Concluding Remarks and Closing (P. Ordejón)

INVITED SPEAKERS

Stefano Baroni, SISSA, Trieste (Italy)

Kieron Burke, Rutgers University, Piscataway (New Jersey, USA)

Mike Gillan, University College London (UK)

Xavier Gonze, Universitè Catholique de Louvain (Belgium)

Richard J. Needs, Cambridge University (UK)

Rubén Pérez, Universidad Autónoma de Madrid (Spain)

Warren Pickett, University of California at Davis (USA)

Rafael Ramírez, Instituto de Ciencia de Materiales, CSIC, Madrid (Spain)

Carme Rovira, Universitat de Barcelona (Spain)

Daniel Sánchez-Portal, University of Illinois at Urbana-Champaign (USA)

David Singh, Naval Research Laboratory (Washington DC, USA)

Magdalena Siodmiak, Philipps Universität (Marburg, Germany)

José Soler, Harvard University (Massachussetts, USA)

Ivo Souza, University of Illinois at Urbana-Champaign (USA)

Nathalie Vast, Commissariat à l'Energie Atomique (France)

Chris van de Walle, Xerox Palo Alto Research Center (California, USA)

Erich Wimmer, Materials Design, s.a.r.l. (Le Mans, France)

Björn Winkler, Universität Kiel (Germany)

Kazuhiro Yabana, Tsukuba University (Japan)

OTHER PARTICIPANTS

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Kiyoyuki Terakura, NIAIR, Tsukuba (Japan)

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Jorge Iñiguez, Universidad del País Vasco, Bilbao (Spain)

Javier Junquera, Universidad Autónoma de Madrid (Spain)

Maider Machado, Universidad del País Vasco, San Sebastián (Spain)

José Luis Martins, INESC, Lisbon (Portugal)

Miguel Moreno, Universidad de Cantabria (Spain)

Alfonso Muñoz, Universidad de La Laguna, Tenerife (Spain)

Jorge Pacheco, Universidade de Coimbra (Portugal)

Rampi Ramprasad, Motorola FPD, Phoenix, AZ (USA)

J. Manuel Recio, Universidad de Oviedo (Spain)

Agustín Válgoma, Universidad del País Vasco, Bilbao (Spain)

Jun Wang, Motorola PSRL, Phoenix, AZ (USA)

ABSTRACTS OF INVITED TALKS

Combination of Electronic Structure Methods and Large-scale Data Analysis: A Tool for Understanding and Innovation

Erich Wimmer and Jürgen Sticht
Materials Design s.a.r.l., Le Mans, France

John Harris
Forschungszentrum Jülich, Germany

Alexander Mavromaras
Institut Supérieur des Matériaux du Mans, Le Mans, France

John Rodgers and Paul Saxe
SciCo Inc., Oceanside, California, USA

Several remarkable scientific and technological developments in the area of materials science are opening new dimensions for research and discovery: (1) Electronic structure methods based on density functional theory allow automatic structural optimization and property predictions for systems of increasing complexity, (2) the algorithmic and numerical robustness of present electronic structure programs allows automatic calculations on a large number of systems, (3) computer processor speed, memory size, and disk storage capacity continue to evolve at an amazing rate while the cost of computing decreases, (4) automation in high-throughput experimentation in conjunction with combinatorial materials science are generating a wealth of experimental data at an unprecedented rate. In the face of these exciting developments, we have started to explore the possibility to combine electronic structure methods and materials databases, thereby expanding the size and scope of existing, purely experimental databases. By comparing calculated results such as crystallographic parameters with those available in experimental databases, it is possible to estimate the uncertainty of computed data. The computational environment used for these investigations is MedeA (Materials Exploration and Design Analysis), which offers, at present, the largest available structural database of intermetallic compounds and two electronic structure programs, namely ”ElectrA” (an augmented spherical wave method) and ”OresteS” (a full-potential linearized muffin-tin orbital method) in the form of an integrated PC-based implementation. As an example of the above mentioned approach, we present preliminary results on lattice optimizations and electronic structure calculations on approximately 5000 existing as well as combinatorially created new compounds. This computed set of data enables a search for novel materials with (a) specific lattice constants and (b) specific electronic properties (e.g. semiconductivity). A perspective on future developments will conclude this contribution.

Fixed-node diffusion quantum Monte Carlo calculations of excited states

R. J. Needs
TCM Group, Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

The fixed-node diffusion quantum Monte Carlo method provides a powerful technique for calculating the energies of both ground *and* excited states. Some basic theoretical considerations will be presented [1], along with several examples of applications to real systems. Calculations of the bandstructure of diamond [2] show good agreement with experiment for the low-lying excited states, although the energies of higher-lying states are overestimated. Calculations on small $\mathrm{Si}_x\mathrm{H}_y$ clusters [3] using a multi-determinant representation of the excited state wave functions are presented. We also present DMC calculations of the ground and excited state energetics of the neutral vacancy defect in diamond [4]. For the ground state we obtain the ^1E state in agreement with experiment. The calculated energy of the lowest dipole allowed transition is consistent with the experimentally observed GR1 band, which has long been identified with the neutral vacancy in diamond, although no previous first-principles *ab initio* calculation of this transition exists. The calculated multiplet splitting of over 2 eV indicates the importance of a proper treatment of electron correlation in this system.

1. W. M. C. Foulkes, R. Q. Hood, and R. J. Needs, Phys. Rev. B **60**, 4558 (1999).
2. M. D. Towler, R. Q. Hood and R. J. Needs, submitted to Phys. Rev. B.
3. A. R. Porter, M. D. Towler, and R. J. Needs, unpublished.
4. R. Q. Hood, P. R. C. Kent, R. J. Needs, G. Rajagopal, and P. Briddon, unpublished.

Polarization and Localization in Insulators: Generating Function Approach

Ivo Souza
Department of Physics and Materials Research Laboratory
University of Illinois at Urbana-Champaign, Urbana, IL 61801-3080 USA

In the last decade there have been significant developments in the theory of insulators. First and foremost is the Berry's phase theory of polarization [1,2,3]. This theory provides the answer to the following seemingly innocuous question: given the ground state wavefunction of a periodic insulating crystal, what is the average bulk macroscopic polarization ? The Berry's phase formula has become a standard tool in electronic structure calculations, and has been successfully applied to a wide range of problems (e.g., ferroelectricity, infrared absorption by amorphous semiconductors, liquid water, and systems under high pressure, phase transitions in correlated lattice models, etc.)

Recent work has indicated that another basic property of insulators which is closely related to electronic polarization is electronic localization [4,5,6]. In Refs. [5,6] the ideas from the Berry's phase theory of polarization were extended in order to address this issue. The work presented in this talk [7] is a contribution to this ongoing effort. In particular we show what is the connection between these recent ideas and the basic notion of localization in the insulating state, introduced by Kohn [8], as well as with the little known work of Kudinov [4].

Our starting point is the following question: given the ground state wavefunction of a periodic insulating crystal, what is the full quantum-mechanical distribution of the bulk macroscopic polarization ? We introduce a cumulant generating function which yields, upon successive differentiation, all the cumulants and moments of the probability distribution of an appropriately defined center of mass $\mathbf{X}/N$ of the electrons in an extended system with N electrons in a periodic volume V. This formulation is able to describe in appropriate limits both the Berry's phase [1,2] and the "single-point" type of formulas [6,9,10]. In the case of the first moment, the average polarization $q_e\langle\mathbf{X}\rangle/V$, we recover the Berry's phase expression. The second cumulant, the mean-square fluctuation of the polarization, can be used to define a localization length ξ_i for the electrons along each cartesian direction: $\xi_i^2 = (\langle X_i^2\rangle - \langle X_i\rangle^2)/N$. It follows from the fluctuation-dissipation theorem that as $V \to \infty$, ξ_i diverges for a metal and is a finite, measurable quantity for an insulator [4].

The present formalism can be recast in terms of Kohn's theory of the insulating state [8], in which the many-electron insulating wavefunction Ψ breaks up into a sum of functions, $\Psi = \sum_{-\infty}^{+\infty} \Psi_{\mathbf{M}}$, which are localized in disconnected regions of the high-dimensional configuration space. It is in this sense that electrons are localized in an insulator, and the desired distribution of the center of mass, $p(\{X_i\})$, is that for the N electrons calculated from the partial wavefunction $\Psi_{\mathbf{M}}$ in one disconnected region. We show that Kohn's functions $\Psi_{\mathbf{M}}$ can be viewed as maximally-localized "many-body Wannier functions", in close analogy with the maximally-localized Wannier functions for non-interacting electrons [5]. The width along the i-th direction of the distribution $p(\{X_i\})$ is $\sqrt{N}\xi_i$; for non-interacting electrons $\sum_{i=1}^{3} (\xi_i)^2$ is a lower bound to the average quadratic spread of the occupied Wannier functions. The quadratic polarization fluctuations have a geometrical interpretation in terms of a metric [5,11] (distance between nearby states) on a manifold of quantum states parametrized by the twisted boundary conditions.

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First-principles calculations of defects and impurities in GaN, AlN, and InN

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A thorough understanding of the behavior of point defects and impurities is of the utmost importance for technological applications of semiconductors. Shallow impurities enable the doping that controls conduction through semiconductor devices. Deep-level impurities as well as native point defects may act as recombination centers, or as sources of compensation that counteract the intended doping. First-principles computations based on density-functional theory and *ab initio* pseudopotentials have significantly contributed to our understanding of defects and impurities. Results for band structure have provided insight into the levels introduced by the point defects; investigations of charge densities and wave functions have illuminated the interaction between the defect and its environment; and calculated total energies have been used to predict defect concentrations and impurity solubilities.

I will illustrate the power of the first-principles approach with a number of recent results for III-nitride semiconductors. We have calculated all the native point defects in GaN [1,2], AlN [3], and InN [4], finding that o nly vacancies have low enough formation energies to occur in significant concentrations. Nitrogen vacancies are *not* responsible for *n*-type conductivity, as has often been assumed; this conductivity therefore has to be attributed to unintentionally incorporated impurities. Nitrogen vacancies *do* play an important role, however, in compensating *p*-type material. Limitations on hole concentrations are still an important problem in the nitrides, and

I will discuss the various approaches we have examined to address this issue. These include a detailed investigation of the role of hydrogen in *p*-type doping [5], as well as an examination of a wide variety of candidate acceptors [6].

I will also devote some attention to the limitations of density-functional theo ry for calculating defects in semiconductors. We have found that the use of the generalized gradient approximation offers no improvement over the local density approximation (LDA) [4,7]. Our main uncertainties result from the band-gap error. I will illustrate how we assess the effects of the band-gap error, and how we ensure that our qualitative conclusions are not affected. For defects in InN, we have compared the defect electronic structure obtained using LDA with the recently developed self-interaction and relaxation-corrected (SIRC) pseudopotential treatment of Vogel *et al.* [8]. The insights gained from this comparison confirm that the general conclusions obtained from the standard LDA calculations remain valid.

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Gas Phase Reactions in Chemical Vapor Deposition of Transition Metal Compounds

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Gas phase reaction mechanism and chemical kinetics are essential components in construction of a computer model for a CVD reactor simulation. Knowledge of nature, thermochemistry and kinetics of critical reactions leading to the film deposition and to byproducts formation help also in the search for obtaining high quality thin films with best chemical, electrical, structural and mechanical properties. A high demand for new films, which can provide superior device properties over existing Si/SiO_2 technology, has stimulated research in a broad area of transition metal based compounds, insulators and (semi) conductors. In many cases very limited knowledge of deposition chemistry is available for potentially interesting compounds.

Two reaction systems will be demonstrated to provide examples of our research on gas phase chemistry $TaCl_5/H_2O$ and $TiCl_4/NH_3$, which are relevant for Ta_2O_5 and TiN CVD, respectively. Quantum chemical calculations at the Hartree-Fock, B3LYP, MP2 and CCSD(T) levels of theory combined with effective core-potentials were performed to investigate initial reactions of $TaCl_5$ with H_2O and ammonolysis of $TiCl_4$. In the latter case we have also investigated the reaction kinetics using TST and RRKM theory. In both reaction systems intermediate Lewis type complexes are formed at lower temperatures in the gas phase and may be responsible for initial adsorption of precursors. Recomendation have been made to avoid formation of $TiCl_4$:NH_3 adducts and their deposition on the reactor walls. Our results provide key thermochemical values for both studied systems. We also explain incomplete ammonolysis of $TiCl_4$ in gas phase and in liquid ammonia.

The thermochemical and kinetic data obtained in our study are currently applied at Motorola for ractor modeling and process optimization.

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The atomic structure and vibrational properties of icosahedral B_4C boron carbide

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Covalently bonded solids based on boron, carbon or nitrogen comprise the hardes t materials presently known. Among them, B_4C boron carbide shows a pecul iar atomic structure composed of $B_{11}C$ icosahedra allowing a sixfold coordination. However, the location of carbon within the boron icosahedron is presently beyond X-ray and neutron diffraction ability.

In this work, the Raman and infrared spectra of icosahedral B_4C boron carbide have been determined by accurate first-principles calculations based on density-functional perturbation theory [1]. Our results account for all the features observed experimentally, including the characteristic

Raman-active mode at 534 cm^{-1}, which is attributed to the libration of the icosahedra, and had been previously identified in icosahedral α-B_{12} boron[2]. A comparison of the calculated vibrational spectra of three possible atomic structures with experimental data allows the first unambiguous determination of the atomic structure of B_4C [3].

Analysis of our data shows that the high bulk moduli of α rhombohedral boron and of B_4C boron carbide - 220 and 240 Gpa, respectively - are mainly determined by the stiff intra-molecular bonding within each icosahedron. This finding is at variance with the current interpretation of recent neutron-diffraction data on B_4C [4] in terms of a postulated larger stiffness of the inter-molecular bonds in icosahedral solids (*inverted molecular compressibility*). Our results show that icosahedral boron-rich solids should be considered as members of a new class of covalently bonded materials.

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Using Density Functional Calculations to Find New Thermoelectric Materials

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Thermoelectric materials are characterized by a dimensionless combination of electrical and thermal transport parameters, known as the figure of merit, $ZT = \sigma S^2 T/\kappa$, where σ is the electrical conductivity, S is the thermopower, T is the temperature, and κ is the thermal conductivity. The best known materials have $ZT \sim 1$ but higher ZT would mean higher energy efficiency in thermoelectric devices. Discovery of new materials with substantially higher ZT near room temperature or below would have important technological ramifications for active cooling of electronics and thermal management.

A good thermoelectric must satisfy the apparently contradictory requirements of high electrical conductivity, like a metal, high thermopower like a doped semiconductor and low thermal conductivity like a glass. Carriers should be weakly scattered to give high σ, but there should be strong scattering of heat carrying phonons.

An additional complication in the search for new high ZT materials comes from the fact that the electrical electrical transport properties (σ and S) are generally very strong functions of the carrier density, so it is not always evident whether or not a given phase is useful as a thermoelectric if only a few samples are studied. In spite of these difficulties at least two new high ZT materials have been discovered in the past few years.

In this talk, I discuss the use of first principles theory to unravel the physics that gives rise to high ZT, both from the point of view of electronic transport and from that of lattice thermal conductivity. This is done mostly using examples of skutterudites and filled-skutterudites. Band structures are used to extract information about electronic transport using kinetic transport theory. Information relevant to heat conduction is extracted using dynamical models constructed from density functional total energy and force calculations.

At the end some new skutterudite compositions are suggested that, if made, may have superior thermoelectric properties to existing materials.

Modeling the ligand binding properties of myoglobin by first-principles molecular dynamics

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Myoglobin, a small globular protein that stores oxygen in muscles, has often served as example of ligand binding, control and recognition. The binding of ligands to its active center (heme) is a complex process determined by many structural and dynamic properties of both the heme and the surrounding protein. Many essential aspects of this function, such as the the way the protein controls the binding of ligands (O_2, CO and NO) or the structure - spin - energy relations at the active center, are a topic of debate [1].

As a first step towards understanding these mechanisms, we will carry out a quantitative study of the properties of the myoglobin active center and its interaction with the O_2, CO, and NO ligands, by means of Car-Parrinello molecular dynamics. The active center is modeled by FeP(Im)(XY) systems (FeP = iron-porphyrin; Im = imidazole; XY = O_2, CO or NO). We will investigate its structure, the energy associated to small deformations, and their relation with the binding energy of the Fe-XY bonds. The dynamical motion of the ligand and its preferential conformations will also be analyzed: while the CO ligand undergoes an essentially harmonic dynamics around its linear equilibrium position, the O_2 ligand prefers a conformation where the O-O axis projection on the porphyrin plane bisects one of the porphyrin quadrants. However, it "jumps" from one porphyrin quadrant to another one every 4 - 6 ps [2]. Finally, a combined QM/MM methodology [3] will be used to investigate the heme-protein interaction.

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SIESTA applications: from biomolecules to liquid surfaces

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The SIESTA method [1] is a powerful code for general-purpose density functional calculations. Using flexible LCAO basis sets and order-N methods, it is aimed mainly to very large systems and high computational speeds. Still, it is also capable of very accurate calculations, at the expense of a higher cost, what makes it specially versatile.

I will describe some recent applications ranging from the *ab initio* study of structural and electronic properties of DNA, to the molecular dynamics simulation of the liquid silicon surface [2]. In the latter, we find a pronounced atomic layering, characteristic of metallic surfaces. However, the analysis of atomic pair correlation functions shows that, unlike in other metals, the layering originates from characteristic surface configurations in which the bonds are partially covalent and directional.

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Applications of Siesta to metallic systems: gold monatomic wires and zintl manganites

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In this talk I will present two recent applications of the SIESTA method [1,2] to the study of the structural and electronic properties of metallic systems.

In the first part, I will present a study [3] of the structural and elastic properties of monatomic gold wires. The equilibrium configuration, for both the infinite wire and short chains of atoms suspended between gold tips, is found to have a zigzag shape which remains under tension. The structure becomes linear only just before breaking. Furthermore, for some lengths, the zigzag chainlike shape is stable even for the free-standing clusters. The stabilization of the zigzag structure can be explained as a result of the transverse quantization of the levels in the wire. This is illustrated with a simple free-electron model. Our calculations also indicate that, at room temperature, the suspended wires could spin around the axis determined by the tips, providing a possible explanation for the extremely long apparent interatomic distances shown by electron microscopy [4].

In the last part of the talk, I will briefly discuss some calculations for the zintl phase manganites, $Ca_{14}MnBi_{11}$ and $Ba_{14}MnBi_{11}$ [5]. These compounds show an unusual magnetic behaviour, but their 104 atoms unit cell has precluded any previous first principles study. We find a gap between the bonding valence bands and the antibonding conduction band. However, the valence bands lack one electron per formula unit to be filled, and the compounds can be characterized as low carrier density *p*-type metals. The Mn atom is magnetic with a moment of 4.5-4.6 μ_B. $Ca_{14}MnBi_{11}$ is found to be ferromagnetic as observed, while for $Ba_{14}MnBi_{11}$ (antiferromagnet with T_N=15 K) ferro- and antiferromagnetic states are calculated to be essentially degenerate. The band structure of the ferromagnetic states is very close to a half-metallic situation.

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First–Principles Simulations of Tip–Surface Interactions on Semiconductor Surfaces

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Understanding the physical processes that occur when two materials are brought together is important to many basic and applied problems as adhesion, friction, wear, fracture and the determination of the elastic and plastic response of materials. The high lateral resolution of the tip–based microscopes, Scanning Tunnelling Microscope (STM) and Atomic Force Microscope (AFM), have made possible to obtain information relevant to those processes on an atomic scale. The interpretation of these experiments requires a detailed knowledge of the tip-sample interaction. During the last few years, we have used first principles methods to gain insight into different regimes of the tip–sample interaction with simulations of processes like nanoindentation[1], diamond polishing[2] and the image formation in the Non-contact AFM (NCAFM), which will be the main topic of this contribution.

Atomic resolution with NCAFM operated in the frequency modulation (FM) detection mode was recently shown to be feasible on the Si(111)–7×7 surface[3]. Since this pioneering work, different reactive semiconductor surfaces as the InP(110), GaAs(110), InAs(110) and Si(100)–c(4×2) have been imaged with this technique.

Theoretical studies[4-9] have started to shed light on the imaging mechanism of the FM-NCAFM and on the delicate nature of the tip–surface interactions. Our first results[4] revealed that the short–range chemical tip–surface interaction plays a fundamental role in the explanation of the atomic resolution capabilities of the FM-NCAFM.

The theoretical analysis of the experimental results is rather complicated because the dynamic nature of the process makes it difficult to relate the measured frequency shift to the properties of the tip–surface interaction. In our approach we combine the displacement curves on the different surface atoms and lateral scans along a number of directions on the surface unit cell, which provide qualitative insight into the NCAFM experimental images, with the use of canonical perturbation theory and our computed tip–surface forces to obtain a direct quantitative comparison with the experimental frequency shifts.

In this contribution, Total–Energy pseudopotential simulations of the short–range (< 5 Å) tip–surface interactions on different semiconductors surfaces (GaAs(110), InP(110) and Si(100)–c(4×2)) with a Si tip are presented. This surfaces provide very stringent tests to the resolution capabilities of the technique, the role of the induced deformations in the tip and sample, and the relative importance of geometric and electronic effects in the image contrast.

Total energy and normal force displacement curves show pronounced deviations from a simple bonding situation. We observe a very significant surface response –related to counterrelaxation of the anion and cation on the (110) III-V surfaces, and dimer flip on the Si(100)–, which leads to a very complicated behaviour of the energy and force curves. Close to contact (< 2 Å), our calculations on the cation of the III-V (110) surfaces show the onset of large lateral forces on the tip apex, which significantly modify the tip structure, well before large repulsive normal forces appear. These lateral forces are due to the interaction of the tip dangling bond with the neighbouring anions, which becomes relevant even for sharp tips as the ones considered here. While similar in many aspects, GaAs and InP(110) surfaces present some significant differences in their interaction with Si tips. The most relevant one is the jump of the Ga atom, with a normal displacement of 1.1 Å towards the tip, for a tip-surface distance of 3.3 Å and the complicated hysteretic behaviour upon tip retraction, which is absent in the InP (110) surface.

Lateral scans at constant tip height for different directions along the unit cell and two values of the tip-surface distance,typical for very weak and stronger "chemical" tip–surface interaction, have been performed. Our results show that force minima close to, but not necessarily coinciding with the atomic positions, provide insight into (1) the reason why only the anion sublattice is experimentally observable in NCAFM on the III-V (110) surfaces, (2) the experimental conditions in NCAFM where the two Si atoms in a dimer can be resolved on the Si(100)–c(4×2), and (3) the simultaneous imaging at one sample voltage of both As and Ga atoms in recent near–contact STM experiments.

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Magnetoelectronic Character of a Superconducting Cuprate

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The coexistence of ferromagnetism with (singlet) superconductivity over any substantial range of temperatures has long been thought to be an impossibility. The discovery by Tallon and coworkers [1] of the ruthenocuprate $RuSr_2GdCu_2O_8$, which is ferromangetic below 132 K and superconducting below 40 K, thus raises many questions. Various experiments place the magnetism in the Ru layer, and the superconductivity in the Cu layer of the $YBa_2Cu_3O_7$-related structure. The internal field of 700 G (based on the measured moment of 1 μ_B per Ru) is of little concern, either as a cause of orbital currents or due to spin splitting. However, the exchange splitting in the RuO_2 layer is likely to be ∼1 eV, and the induced exchange (spin) splitting in the cuprate layers is the first important question to answer.

Based on local density approximation (and generalized gradient approximation) calculations and relying on the inhomogeneous (layered, quasi-2D) crystal, electronic, and magnetic structures, we have been able understand how coexistence of ferromagnetism and superconductivity is possible.[2] An important feature is the weak coupling between the Ru t_{2g} orbitals, which carry the magnetization, and the Cu $d_{x^2-y^2}$ orbitals that we presume to support the superconductivity as in other cuprates. The induced exchange splitting on the Cu-O layers is roughly 25 meV; the precise value is probably dependent on the Ru-O structural distortion, which has only lately been determined. This value is comparable to the expected superconducting gap — not so large as to preclude superconductivity, but perhaps large enough to induce an inhomogeneous superconducting order parameter. The symmetric Cu-O bilayer Fermi surface is the most favorable for supporting a superconducting gap.

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Magnons in real materials from density-functional theory

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We present an implementation of the *adiabatic spin-wave dynamics* which allows to decouple the spin and charge excitations of a many-electron system using a generalization of the adiabatic approximation. The only input for the spin-wave equations of motion are the energies and Berry curvatures of many-electron states describing frozen spin spirals. The latter are computed using a newly developed technique based on constrained density-functional theory, within the local spin density approximation and the pseudo-potential plane-wave method. Calculations for iron show an excellent agreement with experiments.

Dynamical properties from equilibrium path integral Monte Carlo simulations

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In the path integral formulation of statistical mechanics Feynman defined a quantity, the effective classical potential (ECP), as a variational approximation to study static properties of quantum systems in thermodynamic equilibrium. With the formulation of the quantum transition-state theory,[1] Gillan showed that the ECP concept can be also applied to study kinetic properties, i.e. rate constants of thermal activated processes at temperatures were quantum effects are important. Further efforts led to the formulation of centroid molecular dynamics,[2] which aims at the calculation of dynamical properties associated to the nuclei of molecules or solids from trajectories generated by classical equations of motion of particles moving in the ECP. Unfortunately, the range of validity of the latter approach has not been clearly established.

We have recently presented the Schrödinger formulation of the ECP,[3] showing that it is related to the response of the quantum system to static external forces. The static response of the system to these influences, i.e. the static isothermal susceptibility, can be readily extracted from equilibrium path integral Monte Carlo simulations. For many-dimensional quantum systems this susceptibility takes the form of a second rank tensor whose diagonalization provides direct information on the excitation energy of the system. After presenting the physical justification of this new approach, we apply it to study the anharmonic vibrational frequencies of several molecules for which highly accurate potential energy surfaces have been previously derived by ab initio electronic structure calculations. The accuracy of the approximation is studied as a function of both the temperature and the discretization employed in the path integral simulations. The method can be applied to study anharmonic vibrational frequencies of both molecules and solids.

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Excitation energies from Density Functional Theory

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Density-functional theory (DFT), as proposed by Hohenberg, Kohn and Sham [1], has been highly successful in the analysis of interacting-particle *ground states.* Many efforts have also been devoted to DFT-based schemes for *excited states.* Recently, the feasibility of direct excitation-energy computations relying on Time-Dependent Density Functional Theory (TD-DFT) has been demonstrated for atoms, small molecules and clusters [2-5].

In the first part of the presentation, conceptual aspects of TD-DFT are considered. Specific matric elements of exchange and correlation kernels in TD-DFT are computed. The knowledge of these matrix elements not only constrains approximate time-dependent functionals, but also helps to understand the connection between practical approaches to excited states, based either on density-functional theory or on many-body perturbation theory, despite the approximations that have been performed to derive them.

Then, the TD-DFT is applied to the computation of excited state potential energy surfaces. For the $(\mathrm{HeH})^+$ system, we investigate the ground state as well as the 5 lower-lying singlet and triplet Σ states, for a series of internuclear distances. The TD-DFT potentials and kernels are obtained within the (Adiabatic) Local Density Approximation (LDA) as well as within the exchange-only Optimized Effective Potential approximation (TD-xOEP).

For this system, comparison with Configuration Interaction (CI) data shows that, in contrast to the LDA potential, the xOEP potential is reliable enough for the description of the dissociation procedure and the position of avoided crossings between the different excited-state curves. We then present preliminary results obtained with a hybrid TD-kernel recently developped by Burke, Petersilka and Gross. We also compute excited state energies within the ΔSCF approach, using both LDA and GGA.

X.G. acknowledges financial support from the A. von Humboldt foundation and the FNRS (Belgium).

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Real-time method for optical response of clusters and molecules

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The time-dependent density-functional theory (TDDFT) has been developing as an extention of the static density-functional theory to treat the dynamic electronic motion such as excitations and collisions. A simple adiabatic approximation in which the same exchange-correlation potential as static one is used for the time-dependent dynamics has been found to describe rather well the excited state properties.

We have developed a real-time computational method to calculate efficiently the optical responses of finite systems such as clusters and molecules in the TDDFT[1]. In the method, we solve the time-dependent Kohn-Sham equation explicitly in real-time and -space. The frequency-dependent polarizability is then obtained by the time-frequency Fourier transformation of the polarization. The computational demand of our method scales quadratically in system size. This relatively low scaling property allows us to calculate responses of the systems with a few hundred electrons employing the first-principle Hamiltonian.

In my talk, I first explain our numerical method and discuss its advantageous aspects. I then show some applications of our method for optical responses of several finite systems; the collective electronic excitations in metallic clusters, absorption spectra of organic molecules and fullerene, and the optical activity of chiral molecules[2,3].

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Development of time-dependent density functional theory

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Time-dependent density functional theory (TDDFT) is rapidly evolving as a useful tool in quantum chemistry [1], solid-state physics[2], and atomic physics[3]. I'll report progress in my group on the development of TDDFT [For a review, see 4], mostly for finite systems. TDDFT allows the treatment of electrons in response to time-dependent external fields. There are two distinct applications we focus on: Optical response of materials and matter in intnse laser fields.

In the linear response regime, TDDFT is being used to calculate the true excitations of systems from the Kohn-Sham eigenvalues. This involves two distinct approximations: the ground-state energy approximation, whose functional derivative determines the ground-state potential, and the approximation to $f_{\rm XC}$, the XC kernel needed in the TD response equations. I will discuss the accuracy of both these approximations, and a new hybrid for $f_{\rm XC}$. I will also discuss Görling-Levy perturbation theory for the excited-state energies, and the accuracy of Kohn-Sham oscillator strengths.

In a second, more general application, I will talk about matter in intense laser fields, where perturbative methods cannot be applied. I will discuss some fundamental theorems, and the first 3-D exact time-dependent Kohn-Sham calculation[4]. I also hope to discuss the initial-state dependence of TD density functionals, and the accuracy of the adiabatic local density approximation (ALDA) for fully time-dependent problems.

This work is supported by the NSF grant CHE-9875091, and by the Petroleum Research Fund, and by NATO. Collaborators include Neepa Maitra and Paul Hessler at Rutgers, and Heiko Appel, Martin Petersilka, and Hardy Gross at Würzburg. Much material is available from my website, http://crab.rutgers.edu/∼kieron.

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Recent advances in ‘Computational Crystallography / Mineralogy’

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The availability of efficient DFT-based computer codes which allow full-geometry relaxations of low symmetry structures has led to an increasing number of studies addressing questions of interests to crystallographers and mineralogists [1]. The main advantages of using quantum mechanical models are (i) that they can be used to calculate structure-property relations which cannot be obtained by experiments, (ii) that they allow an unambiguous correlation between a structural model and spectroscopic data and (iii) that they can be used to construct polymorphs which have not yet been synthesized, thereby widening the data base from which structure-property relationships can be inferred.

We have exploited the predictive power of parameter-free quantum mechanical calculations in our recent work on the *systematic* prediction of sp^2-hybridised carbon polymorphs [2]. In these studies, a graph-theoretical approach based on labeled quotient graphs was used to enumerate all possible framework structures with less than 6 atoms per primitive unit cell, which were all bonded to three neighbors. These topologically distinct structures were then used as trial structures in DFT-GGA based calculations. After full-geometry optimizations, we could predict structural parameters, physical properties and binding energies.

Further recent applications of DFT-based calculations which will be discussed include the calculation of the energetics of structures with domain walls, and of the pressure-dependence of structures with ordered vacancies (‘Suzuki’-phases).

In ‘Computational Mineralogy’, quantum mechanical models are currently mainly used to understand and predict pressure-induced structural changes of minerals. While in the recent years the main emphasis was placed on studying structurally simple phases present in the Earth’s lower mantle and core, there is now an increasing interest to study the more complex phases present in the upper mantle and the crust.

We have begun to study in detail the compression behavior of garnets, which are important minerals in the Earth’s mantle. With our calculations we could unambiguously identify the compression mechanism of silicate garnets [3] and clarify the interatomic interactions in pyrope [4]. The latter study showed the anisotropy and the anharmonicity of the potential experienced by the ‘small’ Mg-atom which occupies a ‘too large’ dodecahedral coordination polyhedron. Thereby, we could resolve conflicting interpretations of diffraction and spectroscopic data.

I would like to thank my co-workes V. Milman (MSI), L. Akhmatskaya, R. Nobes (Fujitsu) and C. Pickard (Kiel). These studies have been supported by the German Science Foundation (DFG).

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Ab Initio Free Energies and the Composition of the Earth's Core

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The Earth's liquid outer core and its solid inner core consist mainly of iron. However, the density of the outer core deduced from seismic measurements is $6 - 10$ % lower than that of pure liquid iron, so that light impurity elements must also be present. There appears to be a smaller, but still detectable, impurity content in the inner core. Cosmochemical and geochemical arguments show that the impurities are most likely to be S, O or Si, but controversy has continued for 40 years about which of these impurities is dominant. This is a very important question for three reasons: (i) the nature and amount of the impurities affect the depression of freezing point of iron, and hence the temperature at the inner-core/outer-core boundary; (ii) convection in the outer core is believed to be driven by the partitioning of impurities between liquid and solid; (iii) the nature of the impurities has strong implications for the way the Earth and its core were formed 4.6 billion years ago.

Following ideas initially proposed by Car and Sugino [1], we have recently developed methods for calculating the free energy of solids and liquids using first-principles methods [2]. The methods, based on thermodynamic integration combined with carefully constructed reference systems, allow the calculation of free energies with the very high precision needed to obtain accurate melting curves, and we have reported the complete melting curve of pure iron for pressures going up to values (*ca.* 350 GPa) found in the Earth's core [3]. The methods allow one to reduce technical errors in the free energy due to size effects and k-point sampling to the level of a few meV per atom.

In this talk, we describe how we have extended these free energy methods to calculate chemical potentials in multi-component liquids and solids. For the liquid, we use thermodynamic integration, following a path in which iron atoms are continuously transmuted into impurity atoms. This requires simulations in which, for given atomic positions at any instant of time, two separate first-principles calculations are done, corresponding to the two chemical compositions. The energy and forces are then a linear combination of those obtained in the two calculations. In the solid, we use a combination of harmonic calculations, thermodynamic integration and

Monte Carlo shuffling of atoms. We present preliminary results for the cases of S and O dissolved in Fe, which indicate that S is very soluble in the inner core, whereas O shows strong partitioning between solid and liquid. Comparison with seismic measurements indicates that the major impurity in the Earth's core cannot be S, but could be O.

continued...

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ABSTRACTS OF POSTERS

Impurities in Insulator Materials: Influence of the Lattice Relaxation

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The knowledge of the true equilibium distance, R_e, between a Transition-Metal impurity and its neighbours is a prerequisite for a better insight into the origin of new properties due to the impurity cation. As standard diffraction methods are not useful two different approaches have been used for solving that problem: 1) The study of the dependence of EPR and optical parameters on the metal-ligand distance, R. Apart from good information about the actual R_e value, the coupling of electronic excited sates with the A_1 local mode of the system can also be derived from this study. 2) Calculations of the total energy as a function of R.

In the present work both kinds of approach have been followed for exploring a number of systems such as Mn^{2+}, Fe^{3+}, Cr^{3+} [1] or Ni^{+} impurities in fluorides, Cr^{4+} in oxides or more unusual ions such as Ag^0 or Tl^{2+} in halides [2]. As salient feature parameters like the isotropic superhyperfine constant, A_s, the cubic-field splitting parameter, 10Dq, or the energy of charge transfer transitions are found to be particularly sensitive to R variations. For instance in the case of Mn^{2+} and Fe^{3+} in fluorides R_e variations down to 0.05 pm can be detected through the A_e parameter measured by ENDOR spectroscopy. This figure is certainly smaller than the resolution (≈ 2 pm) reached throug h the EXAFS technique. The origin of the strong R dependence of parameters like A_e or 10Dq will be also discussed in detail.

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Electron density in the peptide bonds of crambin

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Crambin is a plant seed hydrophobic protein with 46 residues and 642 atoms. Ultra high resolution X-Ray crystallography recently gave experimental information on the electronic distribution in the protein. Here we present the results of density-functional calculations of crambin in vacuo to study the deformation electron density in its peptide bonds in comparison with the experimental data. The comparison is centered on the average peptide-bond map, where the experimental results are clearest. We then use the theoretical results to ascertain on differences among peptide bonds associated to the different residues they connect and other environmental differences.

Martha Teeter, Victor Lamzin and Robert Blessing are gratefully acknowledged for the diffraction data collection and processing. This work was supported by Spain's DGES through project PB95-0202.

Real-space finite difference Poisson solver in SIESTA

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We have implemented a real-space finite difference Poisson solver in the SIESTA code. While the current solver uses FFT's, the new one uses the conjugate gradient (CG) method. The new implementation handles uniform grids, arbitrary choice of discretization order, and mixed boundary conditions. The advantage of this approach over the previous one are the use of smaller unit cells in cluster calculations and semi-infinite systems, and the ability to solve problems involving charged systems. As an illustration of the method we compare the Kohn-Sham energy, memory usage, and CPU time against unit cell size for an isolated carbon atom and for a C60 molecule, using both CG and FFTs. We also plan to calculate the ionization energy of C60, defined as $E_{\mathrm{C60}} - E_{\mathrm{C60^+}}$, where $E_{\mathrm{C60^+}}$ is the energy of the ionized C60 molecule.

Parallel SIESTA

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The first principles electronic structure code SIESTA [1,2] for performing calculations in a localised basis set has been modified to execute in parallel. Apart from the benefits of increased real time execution, the use of distributed memory allows much larger jobs to be performed than would be possible given the limitations of a single processor. In order to facilitate the parallelisation the code has been modified to use fortran90 for dynamic memory allocation and MPI has been used as the communication mechanism between nodes.

For the present version the parallelisation strategy is targetted at achieving load balancing on modestly parallel machines. Hence the work and data are distributed by orbitals during integral evaluation and diagonalisation using a block cyclic scheme. In contrast the evaluation of terms on the underlying mesh are distributed by a 2-D blocked spatial decomposition. Results will be presented to illustrate the scalability of execution on a Cray-T3E.

This work was funded by the Royal Society and parallel computing facilties were made available by EPSRC through the Materials Chemistry Consortium.

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Density functional calculations of planar DNA base-pairs

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We present a systematic Density Functional Theory (DFT) study of geometries and energies of the nucleic acid DNA bases (guanine, adenine, cytosine and thymine) and 30 different DNA base-pairs. We use a recently developed linear-scaling DFT scheme, which is specially suited for systems with large numbers of atoms. As a first step towards the study of large DNA systems, in this work: (i) We establish the reliability of the approximations of our method (including pseudopotentials and basis sets) for the description of the hydrogen-bonded base pairs, by comparing our results with those of those of former calculations. We show that the interaction energies at Hartree-Fock geometries are in very good agreement with those of second order Møller-Plesset (MP2) perturbation theory (the most accurate technique that can be applied at present for systems of the sizes of the base-pairs). (ii) We perform DFT structural optimizations for the 30 different DNA base-pairs, only three of which had been previously studied with DFT. Our results provide information on the effect of correlation on the structure of the other 27 base pairs, for which only Hartree-Fock geometries were formerly available.

This work was supported by Spain's DGES under grant PB95-0202. P.O. was partially supported by a Sponsored Research Project from Motorola Phoenix Corporate Research Laboratories.

Work function of adsorbate covered graphene edges

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In this study, we focus on the work function of arrays of graphene ribbon edges which are potential electron sources in field assisted electron emission applications. Our calculations are based on density-functional theory within the local density approximation using nonlocal pseudopotentials. A plane wave basis set was used to expand the wave functions, charge density and potentials. The peripheral carbon atoms were assumed to be arranged in a zigzag fashion, and were either unpassivated or terminated with H, O or Cs.

For periodic systems, like the array of graphene ribbons, we find that the work function can be partitioned into two parts: the first being an anisotropic bulk property related to the electron affinity of the material, and the second part depending linearly on the dipole moment per unit surface area. The latter contribution tends to increase the work function if the adsorbate is

more electronegative than the substrate (e.g., oxygen, in the present study), since the net surface dipole moment is increased (relative to the clean surface value) in such cases. Electropositive adsorbates (e.g., hydrogen and cesium) have the opposite effect, and a judicious choice of the adsorbate can ensure a small work function. The former contribution to the work function turns out to be the work function in the limiting situation of zero surface dipole moment, and may be interpreted as the minimum possible work function attainable for a particular surface. In the case of zigzag graphene edges, this value is determined to be 1.4.

Microscopic description of the zinc blende-rock salt phase transition

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We present the results of first principles calculations directed to the investigation of a microscopic mechanism that accounts for the atomic displacements in the pressure induced zinc blende(B3)-rock salt(B1) phase transition. We combine computations using the localized Hartree-Fock *ab initio* Perturbed Ion (*ai*PI) method [1], and non local exchange and correlation functionals within the density functional theory formalism implemented in the CRYSTAL program [2]. The ZnO crystal has been used as the model system. A careful analysis of the symmetry of the nine-parameter (three lattice parameters, three cell angles, and the three coordinates of an internal atomic position) energy Hessian in the B3 phase allows us to propose the transition path (TP). In the TP, the R3m symmetry of a single molecule unit cell is maintained and only three variables, namely the internal coordinate $x = y = z$, the lattice parameter $a = b = c$, and the rhombohedral angle $\alpha = \beta = \gamma$ are needed to describe the mechanism. Despite being 60° in both B3 and B1 phases, α must be considered in the description of the transition path, since otherwise the atomic displacements will lead to unrealistically high energies barriers.

The transition mechanism can be monitored following the change in the internal coordinate from 0.25 (B3) to 0.50 (B1) (crystallographic units). The transition state at the thermodynamic transition pressure ($P_{\mathrm{tr}} \simeq 8$ GPa) is a first order saddle point approximately located at the middle of the path (x =0.375), being the rhombohedral angle close to 70° and the lattice parameter below the equilibrium value at the B1 site. The study of the chemical bonding along the proposed TP explains the increasing of the coordination number from 4 (B3) to 6 (B1): a (0,0,0) ion passes from being a first-neighbor to a third neighbor, whereas three ($\frac{1}{2}$,$\frac{1}{2}$,1) ions, which are third neighbor in the B3 phase, are finally first-neighbor in the B1 structure. Preliminary calculations within the context of the Atoms in Molecules theory [3] predict a seven-fold coordination in specific ranges of the internal coordination during the transition path.

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5.4 Reports on Collaborative Visits

Report on a collaborative visit of Carme Rovira (Universitat de Barcelona, Spain) to the Max-Planck-Institut für Festkörperforschung (Stuttgart, Germany)

Summary

I recently visited the group of Michele Parrinello at the Max-Planck-Institut für Festkörperforschung in Stuttgart (8.11.99 - 21.11.99). The objective of the visit was to finish projects that were started when I was postdoc in this group, and discuss on our recent results on models of the B_{12} coenzyme and hemeprotein dynamics.

On one side, I discussed with M. Kaupp and M. Parrinello on our recent calculations of NMR chemical shift tensors of oxyhemoglobin models. Our calculations are aimed at reproducying the unusually large experimental 17-O_2 chemical shifts of oxyhemoglobin and to explain the temperature dependence of the solid-state NMR spectra. We could relate it to the peculiar anharmonic motion of the Fe-O_2 moiety, as evidenced in our recent MD simulations (Rovira, Parrinello, Biophys. J., in press).

On another hand, I discussed with M. Parrinello on our calculations of structural and electronic properties Co-based complexes related to the B_{12} coenzyme (Rovira, Kunc, Parrinello, in preparation). We also discussed on our ongoing investigation on hemeprotein dynamics. In particular, we are currently investigating the process of ligand binding by means of hybrid QM/MM methods recently developped in the Stuttgart group (Eichinger et al. J. Chem. Phys. 1999). At the same time, I could take the opportunity to pay a short visit to H. Grubmueller (Max-Planck-Institut für Biophysicalische Chemie, Göttingen), who developped the classical MD scheme that can be coupled to the CPMD program of Stuttgart, and to U. Nienhaus (Univ. of Ulm), who is doing investigations on the ligand escaping pathways in myoglobin by means of laser-induced photolysis followed by spectroscopic characterization.

The visit was very fruitful on both sides and I acknowledge the Psi-k network for making it possible.

Carme Rovira

Report on a collaborative visit of G. Madsen (University of Aarhus) to Prof. K. Schwarz and Prof. P. Blaha's group (TU Vienna)

December 1-22, 1999

My visit to Vienna was a continuation of my work on the total electron density in crystalline systems. The aim of my visit was to check whether the presence of non-nuclear maxima(NNM) in the electron density is a real effect, present also in DFT calculations, or an artefact of either the Hartree-Fock method or a basis set problem in LCAO type calculations.

NNM have so far been found mainly in gas-phase model systems. Furthermore they have been reported in the HF densities of solid Li and Na (1) and in the experimental Be density (2). Their existance is very much a matter of discussion in literature. For example they have been shown to be an artefact of the basis-set used for the gas-phase Na_4 cluster (3). Also the presence of NNM in the experimental Be density has been claimed to be an artefact of the method used to derive the electron density (4). Appart from the metallic systems a recent study also reported NNM inside a paramagnetic sodium cluster, which can be formed inside the cages of a host sodalite system (5).

During my visit to Vienna, we have performed highly converged LAPW calculations using the WIEN97 code for some simple metallic systems. We have found that the total electron densities of hcp Be and Mg excibit extremely small non-nuclear maxima. Also bcc Li exhibits a NNM, while bcc Na, contrary to previous reports does not. Inside the sodalite supported sodium clusters very clear NNM were also found.

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Georg Madsen TU Vienna, January 13, 2000

Report on a collaborative visit of P. Korzhavi (Physics Department, Uppsala University) to Prof. R. Podloucky (Department of Physical Chemistry, University of Vienna)

January 17-22, 2000

The visit of P. Korzhavi in Vienna was intended to initiate discussions and possible cooperations between the two groups in Uppsala and Vienna. Both groups are working intensively on defects in intermetallics such as vacancies and antisites with ab-initio techniques and different methods for formulating the thermodynamics. The Uppsala group made an appreciable progress in formulating constitutional and thermal disorder for point defects in a binary alloy in a concise way which we here in Vienna try to combine with our approach. Here in Vienna we performed extensive studies on the migration of atoms which together with the formation described within thermodynamical equilibrium gives the connection to measurable data. P. Korzhavi could also make use of the close collaboration here in Vienna with experimental groups (W. Pfeiler, Inst. f. Mat. Physics, H. Ipser, Inst. f. Anorganic Chemistry) with whom he had intensive discussions. For Ni_3Al, the material we all (including the Uppsala group) are very much interested, a rather high and puzzling activation energy for defect processes was derived from experiment which we believe we understand now -corroborated by the discussion with Korzhavi- in terms of correlated atomic jump processes. It is planned that Korzhavi will provide us with a concept of complete defect interactions for which our elaborate *ab initio* calculations will be further utilized. P. Korzhavi gave also a seminar talk exactly about the subject given in the title which attracted a considerable number of people working in the field.

Summarizing, the visit of P. Korzhavi was very fruitful and we hope to establish a collaboration between the two groups from now on.

R. Podloucky

6 News from CCP9

UK's Collaborative Computational Project 9 on "Computational Studies of the Electronic Structure of Solids"

6.1 Reports on Workshops

6.1.1 Report on COST-TMR-CCP9 Workshop

International Workshop on 'Mesoscopic Superconductors and Hybrid Structures'

Lancaster University, 17-20 December, 1999

Organiser: Vladimir I. Falko (Lancaster)

Co-organisers:Bernard Pannetier (Grenoble) and Colin Lambert (Lancaster)

Sponsors:
European Union Co-operation in Sciences and Technology, Action on Mesoscopic Electronics
Training and Mobility of Researchers Programme on Phase Coherent Dynamics of Hybrid Nanostructures
EPSRC-UK Collaborative Computational Project 9

http://www.lancs.ac.uk/users/esqn/cost-tmr/

A spectacular progress in nano-technology and the recent development of techniques to produce high-quality heterojuctions between different types of metals is now giving birth to a new area of material research: phase-coherent nano-scale hybrid systems made of conventional ferromagnetic (F) and superconducting (S) materials, and normal metals (N). Besides a purely academic interest to understand, how does the superconducting proximity effect transform in a circuit with ferromagnetic components, and under the non-equilibrium condition, which can be generated in the normal part of an S/N/S sandwich, the intense efforts of several UK and European groups (at Royal Holloway (London), CEA-Saclay, CNRS-Grenoble, Delft UT, Groningen UT, Copenhagen

U, etc.) are tempted by the hope to produce physical realization and to study the operation of a controllable π-junction, which is believed to allow one to make a basic building block for the quantum computing hardware. Theoretical predictions of a possibility to realize π-junctions using S/F/S systems (I. Buzdin, V. Bulaevski), or driving the normal metal part of a small S/N/S multilayer far from the equilibrium (A. Volkov), which have anticipated the observations of these effects by about a decade, are now being confirmed experimentally. At the same time, d-wave pairing in HiTc superconductors also gives grounds for the existence of Josephson π-junctions, which represents another area where the hunt for a controllable π-junction design has began.

The Lancaster Workshop has brought together experts in nano-fabrication technology of metals, experimentalists working on transport and magnetic properties of mesoscopic superconductor wires and dots, and theorists modeling Andreev processes in equilibrium and non-equilibrium S/N/S and S/F/S junctions. It has been attended by more than 60 researchers, whose contributions were grouped into five oral sessions and one long poster/discussion session.

Just reflecting the main focus of the meeting, two oral sessions were dominated by discussions of the spin-polarized transport in systems with superconducting and ferromagnetic components. The heart of the problem discussed in several reports (M. Giroud, Yu. Nazarov, F. Sanvito, I. Sosnin, B. van Wees, A. Volkov) consisted in the issue of how to achieve non-quilibrium spin accumulation at the F/S interface or in F/N/S sandwiches. Then, F. Hekking and G. Falci have reported the complete theoretical solution of the problem of a parity effect (even/odd number of electrons in a mesoscopic quantum dot) on the spin polarization properties of superconducting islands. Two other sessions addressed the problems of a proximity effect in disordered metals under the non-equilibrium conditions (B. Hansen, J. Kutchinski, P. Samuelsson), and also to the theory and experimental observations of multiple Andreev scattering processes (R. Taboryski) and the theory of Andreev states in irradiated S/N/S junctions (R. Shekhter). A.Geim (Nejmegen High Magnetic Field Facility) has reported an observation of a new type of non-equilibrium fluxoid state in a micron-size superconducting disk, and M. Sanquer (CENG-Grenoble) has presented the results of the first experimental proof of the shot noise doubling in N/S contacts. One more session has been devoted to the effect of electron-electron correlations and phase fluctuations on the transport in quasi-one-dimensional normal metals and superconductors. The analysis of decoherence efficiency in the Josephson junctions arrays has been represented by J. Siewert, with the aim to assess the limitations in optimisation of parameters in the single and two-qubit design. The recent technological development and the detailed conduction channels analysis metallic atomic contacts was reviewed by C. Urbina (Saclay) and N. Agrait (Madrid).

The MSHS-Workshop has been the first in the series of four narrowly focused meetings planned for the next three years within the EU COST Action on 'Mesoscopic Electronics', in collaboration with other EC Science programmes. This series of meetings is coordinated by the Working Group on Mesoscopic Superconductivity, contact persons: B.Pannetier (CNRS-Grenoble France, email: pannetie@labs.polycnrs-gre.fr) and F.Peeters (University Antwerpten Belgium, email: peeters@uia.ua.ac.be).

The programme and abstracts of talks presented at the Workshop are attached below.

Workshop Programme

December 17

Session Ia: Non-equilibrium and proximity effects in hybrid structure

Chair: M. Buttiker

9.30 R. Taboryski (*Copenhagen*)
Interference effects in diffusive Al/GaAs/Al S/N/S junctions
10.00 M. Sanquer (*Grenoble*)
Shot noise in N/S junctions
10.30 C. Urbina (*Saclay*)
Supercurrent in atomic contact

Session Ib: Non-equilibrium and proximity effects in hybrid structures

Chair: Y. Nazarov

11.20 D. Anghel (*Jyväskylä*)
Trapping of quasiparticles of a non-equilibrium superconductor
11.50 J. Hansen (*Lyngby*)
Photon-assisted Andreev transport and sub-gap structures
12.20 F. Sols (*Madrid*)
Self-consistent theory of transport in superconducting wires

Session IIa: Hybrid systems with normal and ferromagnetic elements

Chair: B. Pannetier

14.30 I. Sosnin (*London*)
Electron transport properties of ferromagnet/superconductor nanostructures
15.00 A. Volkov (*Lancaster*)
Spin polarized transport in mesoscopic ferromagnet/superconductor structures
15.30 B. van Wees (*Groningen*)
Transport in hybrid nanostructures
16.00 R. Shekhter (*Chalmers*)
Andreev states under irradiation

Session IIb: Hybrid systems with normal and ferromagnetic elements

Chair: B. van Wees

17.00 M. Buttiker (*Geneve*)
Distribution functions and current-current correlations in N/S heterostructures
17.30 P. Samuelsson (*Leiden*)
Non-equilibrium Josephson current in multi-terminal S/N/S-junctions
17.50 M. Giroud (*Grenoble*)
Conductance of Ferromagnetic/Superconducting mesoscopic wires
18.20 F.Taddei (*Lancaster*)
Interplay between spin-polarised transport and superconductivity in nanostructures

December 18

Session IIIa: Hybrid systems with normal and ferromagnetic elements

Chair: V. Petrashov

9.15 Yu. Nazarov (*Delft*)
Andreev reflection versus heating near S/F boundary
9.45 J. Aarts (*Leiden*)
π-junctions in S/F systems
10.15 A. Richter (*Hamburg*)
Transport properties of Nb/InAs (2DEG) hybrid structures

Session IIIb: Hybrid systems with normal and ferromagnetic elements

Chair: R. Shekhter

10.40 Z. Szotek (*Daresbury*)
Quasiparticles in High Tc Superconductors
11.10 U. Zuelicke (*Karlsruhe*)
Andreev reflection in strong magnetic fields
11.30 C. Bruder (*Basel*)
The proximity effect in mesoscopic S/N structures
12.00 J. Kutchinsky (*Copenhagen*)
Injection effects in mesoscopic three-terminal S/N junctions
12.20 Poster Session/Discussions
14.30 Poster Session/Discussions/Visit to Lancaster MicroKelvin Laboratory

Session IV: Mesoscopic and non-equilibrium effects in superconductors

Chair: F. Peeters

16.00 A. Geim (*Nijmegen*)
Fine Structure in Magnetisation of Individual fluxoids
16.30 A. Filip (*Groningen*)
Phase coherent transport in superconducting quantum dots
16.50 G. Falci (*Catania*)
Thermodynamic and spectral properties of ultra-small superconducting grains
17.20 F. Kusmartsev (*Loughborough*)
New type of localised excitations in Josephson ladders
17.50 F. Hekking (*Grenoble*)
Re-entrant spin susceptibility of a superconducting grain
18.20 S. Shapira (*Cambridge*)
Conductance anomalies in diffusive S/N junctions

December 19

Session V: Correlations, interactions and mesoscopics

Chair: C. Lambert

9.15 J. Siewert (*Catania*)
Dephasing in tqo-qubits Josephson junction arrays
9.35 R. Smith (*Birminghan*)
Width and magnetic field dependence of Tc in ultranarrow superconducting wires
10.05 A. Zaikin (*Karlsruhe*)
Superconductivity and fluctuations 1D: a new quantum phase transition
10.35 R. Raimondi (*Rome*)
Non-linear conductivity and quantum interference in disordered metals
10.55 N. Agrait (*Madrid*)
Electron-phonon interaction in atomic wires

Abstracts of the Workshop

Transport in hybrid nanostructures

B.J.van.Wees
Applied Physics Department, Groningen University,
Groningen, The Netherlands

General review and report on the recent results on superconducting transistor and the spin-dependent transport in super/normal and semiconductor systems.

Andreev reflection versus heating near SF boundary

Yu. V. Nazarov, A. Braatas, W. Beltzig
Applied Physics Department, Delft University of Technlogy,
Delft, The Netherlands

We present a straightforward model to describe the resistance change at SF boundary. The role of superconductivity is twofold: i) it modifies the boundary resistance and ii) it causes spin accumulation in the ferromagnet. The voltage dependence of the differential resistance is dominated by the heating effect.

Interference effects in diffusive Al/GaAs/Al SNS junctions

Rafael Taboryski
Danish Institute of Fundamental Metrology, Anker Engelunds Vej 1,
Lyngby, Denmark

We discuss measurements on biased flux sensitive interferometers exhibiting a strong modulation in magneto resistance oscillation amplitude as a function of DC bias. The maxima in modulation amplitude coincide with the sub gap structure in the same samples.

Injection effects in mesoscopic three terminal S/N junctions

Jonatan Kutchinsky
Department of Physics, Technical University of Denmark,
Copenhagen, Denmark

We discuss recent measurements showing strong modulation of the critical supercurrent in three terminal SN structures by means of non-equilibrium injection into bound Andreev states in the normal metal.

New type of localised excitations in Josephson ladders

R T Giles and F V Kusmartsev
Department of Physics, School of Mathematics and Physics,
Loughborough University, Leicestershire, LE11 3TU, United Kingdom

We describe localised excitations such as discrete breathers and rotobreathers when a uniform dc current is passed through a single-leg ladder in an applied magnetic field.

Spontaneous supercurrents in superconducting -junction rings

James F. Annett, J.J. Hogan O'Neill
Department of Physics, Bristol University, Bristol, UK

Recently superconducting rings have been counstructed exhibiting half-integer flux quantization. Such rings have a ground state which spontaneously breaks time reversal symmetry and has a ground state supercurrent. Here we develop a microscopic model using a d-wave superconductor in a ring topology containing one or more grain boundary junctions. For a single low angle grain boundary junction we no ground state supercurrent, while for a large angle grain boundary we find a spontaneous supercurrent consistent with the experiments.

The proximity effect in mesoscopic S/N structures

Christoph Bruder
Departement Physik und Astronomie, Universität Basel, Switzerland

In the first part, I review the theory of the magnetic response of superconductor–normal-metal proximity systems for arbitrary impurity concentrations at arbitrary temperatures. In a second part, I report on the local density of states of mesoscopic SN samples.

Electron-phonon interaction in atomic wires

N. Agrait, C. Untiedt, G. Rubio Bollinger, S. Vieira
Laboratorio de Bajas Temperaturas, Dept. Fisica de la Materia Condensada,
C-III Universidad Autonoma de Madrid, 28049 Madrid, Spain

We have measured the electron-phonon interaction in atomic wires of single gold atoms freely suspended between two electrodes. This extremely simple systems makes possible the detailed study of the interaction of electrons with elementary excitations and the mechanisms of dissipation in a one-dimensional system.

Andreev states under irradiation

Robert Shekhter
Applied Physics, Chalmers University of Technology,
SE-412 96 Göteborg, Sweden

We show that transport through a superconducting quantum point contact biased at subgap voltages is strongly affected by a microwave field. The subgap current is increased by several orders of magnitude. Quantum interference among resonant scattering events involving photon absorption is reflected as an oscillating structure in the I-V curve. We also discuss how the same interference effect can be applied for detecting weak electromagnetic signals up to the gap frequency, and how it is affected by dephasing and relaxation.

Conductance of mesoscopic F/S wires

Monique Giroud, Klaus Hasselbach, Herve Courtois, Dominique Mailly, Bernard Pannetier
CRTBT, CNRS- Grenoble, France

We will report on our last measurements on ferromagnetic (F) wires in contact with a superconductor (S). Theconductors geometry was chosen in order to discriminate contributions from interface resistance, parallel resistance of the superconductor, and resistance of the ferromagnetic strip itself.

Charging and charge fluctuations in N/S hybrid systems

A.M. Martin and M. Buttiker
Physics Department, University of Geneva, Geneve, Switzerland

No abstract has been submitted.

Width and magnetic field dependence of T_c in ultra-narrow superconducting wires

Robert A Smith and Beccy S Handy (Birmingham), Vinay Ambegaokar (Cornell)
School of Phsyics and Astronomy, Birmingham University,
Edgbaston, Birmingam, UK

We calculate the dependence of the transition temperature in ultra-narrow wires on width and magnetic field using both standard many-body perturbation theory and a non-perturbative re-summation method. We compare the two theoretical approaches to each other and to experiment.

Nonequilibrium Josephson current in multiterminal S/N/S-junctions

Peter Samuelsson
Lorentz Institut, Leiden University, Leiden, The Netherlands

No abstract has been submitted.

Fine structure in magnetization of individual fluxoids

A.K.Geim (University of Nijmegen, Nijmegen, The Netherlands),
S.V.Dubonos (Chernogolovka), J.J.Palacios (University of Madrid)

Spatial confinement of superconductivity turns the standard magnetisation dependence into a series of discrete magnetisation curves corresponding to different numbers of fluxoids. On top of this dominant quantisation, a fine structure is observed, which we attribute to transitions between different configurations of the same number of vortices and to their merger into a single giant vortex.

Supercurrent in atomic contacts

M.F. Goffman, R. Cron, A. Levy Yeyati*, P. Joyez, M.H. Devoret, D. Esteve and C. Urbina
SPEC, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France
**Departamento de Física Teórica de la Materia Condensada c-V,*
Facultad de Ciencias, Universidad Autónoma de Madrid,
28049 Madrid, Spain

Using microfabricated breakjunctions we have produced Al single-atom contacts and measured the maximum supercurrent they can sustain. Such a contact accommodates three conduction channels, the transmissions of which are determined from the highly non-linear current-voltage characteristics. Once the transmissions are known, the supercurrent is calculated by considering two Andreev bound states per channel. We will compare the predictions of this model with our experimental results.

Non-linear conductivity and quantum interference in disordered metals

Roberto Raimondi
Physics Department, Univ. di Roma Tre, Rome, Italy

We find that an electric field, in disordered conductors, gives rise to dephasing in the particle-hole channel, thus depressing the interference effects due to disorder and interaction and leading to a non-linear conductivity. Relevance for experiments is discussed.

Superconductivity and fluctuations in 1D: a new quantum phase transition

A.D. Zaikin
Institut fuer Nanotechnologie, Forschungszentrum Karlsruhe,
76021 Karlsruhe, Germany

This work addresses a fundamental problem of interplay between superconductivity and quantum fluctuations in ultra-thin metallic wires. We predict a new superconductor-to-metal (insulator) phase transition controlled by dissipation. It appears that our prediction was confirmed in a recent experiment by Mike Tinkham and co-workers.

Conductance anomalies in diffusive SN junctions

Shye Shapira
Cavendish Laboratory, University of Cambridge,
Madingley Road, Cambridge CB3 OHE, UK

We observe a sharp peak in the conductance of a diffusive SN (aluminium/n++ GaAs) junction in a the very close vicinity of T_c. Applying a magnetic field of 14mT we are able to destroy the conductance enhancement, leaving only the resistance enhancement at lower temperatures.

Distribution functions and current-current correlations N/S heterostructures

Markus Buttiker
Physics Department, University of Geneva, Geneve, Switzerland

We discuss the effective, sample specific, non-equilibrum distribution function and current-current correlations in multiterminal hybrid structures by extending the concept of partial density of states. We find that current-current correlations can change sign but only due to a mesoscopic effect.

Self-consistent theory of transport in superconducting wires

Fernando Sols
Universidad Autonoma de Madrid, Madrid, Spain

A self-consistent theory of equilibrium and non-equilibrium superconducting transport is presented, with inclusion -in the equilibrium case- of the electromagnetic equations, which permits the study of the Meissner effect in realistic wires.

Trapping of quasiparticles of a non-equilibrium superconductor

Jukka Pekola, Dragos Anghel
University of Jyväskylä, Department of Physics,
P.O. Box 35 (Y5), 40351, Jyväskylä, Finland

Tunnelling of hot electrons in a SINIS micro-cooler tends to create a non-equilibrium distribution of quasiparticles in the superconductor (S). In our experiments, and theoretically also, we have investigated the influence of placing an extra normal metal electrode (qp-trap) in metal-to-metal contact with the superconductor to be thermalized.

π-junctions in S/F systems

J. Aarts (1), A. A. Golubov (2), V. Ryazanov (3)
(1) Kamerlingh Onnes Lab, Leiden University, Leiden, The Netherlands
(2) Twente University of Technology, The Netherlands
(3) Inst. for Solid State Physics, Chernogolovka, Russia

It has been predicted long ago that the phase of the order parameter can be changed through the ferromagnetic layer in an S/F/S junction. We present the first preliminary experimental results for the existence of such 'π-junctions'.

Quantum computation with Josephson junction qubits

Robert Scovell
Department of Physics, Bristol University, Bristol, UK

Recent nano-fabrication techniques have allowed nanoscopic Cooper-pair boxes to be built which are small enough to have intrinsic capacitances in the femtoFahrad regime. As a result, the energy associated with adding a single Cooper-pair to the box is ~1K. Following the work of Schon et al.[1] and in the light of the very promising experimental results that Nakamura et al. have provided [2], we study the dynamics of these charge systems using a quantised Ginzburg-Landau theory. The hope is that we can develop a scheme for reliable quantum computation using a large array of these boxes which will serve as a quantum register in a quantum computer.

Photon assisted Andreev transport and sub-gap structures

J.B. Hansen (1), M. Wildt (2), J.Kutchinsky (1), R.Taboryski (3),
C.B.Sorensen (2), and P.Lindelof (2)
(1) Dept. of Physics, Techn. Univ. of Denmark, Build. 309,
DK-2800 Lyngby, Denmark
(2) Niels Bohr Institute, Univ. of Copenhagen,
DK-2100 Copenhagen, Denmark
(3) Danish Inst. of Fund. Metrology, Anker Engelundsvej 1,
DK-2800 Lyngby, Denmark

We report on measurements of microwave induced perturbations (”satellites”) of the sub-harmonic energy gap structure in the I-V curves of superconductor-semiconductor-superconductor junctions. The observed behaviour is analogous to photon assisted tunnelling but it is here asociated with multiple Andreev reflections.

Thermodynamic and spectral properties of ultrasmall superconducting grains

G. Falci (1), Rosario Fazio (1), A. Mastellone (1), and F.W.J. Hekking (2)
(1) Dipartimento di Metodologie Fisiche e Chimiche (DMFCI),
Universita di Catania, viale A. Doria 6, 95129 Catania, Italy
(2) University Joseph Fourier, Grenoble, Cedex 9, France

We study the problem of superconductivity in metallic dots. Spectral properties which can be expressed as universal functions allow a quantitative characterization of the crossover to ”superconductivity”. Parity effects in the ground state and the excitation spectrum are discussed. We also study thermodynamic quantities and address the question of the effect of level statistics when measurements on ensammbles of grains are performed.

Re-entrant spin susceptibility of a superconducting grain

F.W.J. Hekking
University Joseph Fourier, Grenoble, Cedex 9, France

We study the influence of parity effects and pairing correlations on the spin susceptibility of a small superconducting grain. In particular we find that the temperature dependence of suscep-

tibility is qualitatively different from standard bulk BCS behaviour.

Spin-polarised transport in mesoscopic F/S structures

V.I. Fal'ko, C.Lambert , and A.F. Volkov
School of Physics and Chemistry, Lancaster, University, LA1 4YB, UK

We study transport properties of mesoscopic ferromagnet-superconductor (F/S) structures. The boundary condition at the F/S boundary are derived in the diffusive limit. Using these boundary conditions, we calculate the conductance of a one- and multiple-domain ferromagnet in a F/S structure. We also study the effect of spin-polarized electrons on the Josephson critical current in a four-terminal S/N/F structure (N is a normal, nonmagnetic metal).

Shot noise in N/S junctions

Marc Sanquer
DRFMC-SPSMS-LCP CEA-Grenoble 17, rue des Martyrs 38054 Grenoble,
Cedex 9, France

We report on the first observation of the doubled shot noise in a Nb-Cu junction.

Interplay between spin-polarised transport and superconductivity in hybrid nanostructures

Fabio Taddei, Stefano Sanvito and Colin J. Lambert
Physics Department, Lancaster University, Lancaster, LA1 4YB, UK

We examine current-perpendicular-to-the-plane giant magnetoresistance (GMR) in magnetic multilayers and show that in the absence of spin-flip scattering, replacing one of the normal contacts by a superconductor dramatically reduces the GMR ratio. Results in the presence of spin-orbit scattering and non-aligned moments are presented, both of which are shown to restore GMR.

Quasiparticle-phonon down-conversion in superconductos

A.G.Kozorezov, A.F.Volkov and J.K.Wigmore
Department of Physics, Lancaster University, Lancaster, LA1 4YB,UK

We have developed a theory of quasiparticle and phonon energy down-conversion in non-equilibrium superconductors following the absorption of an energetic photon. This stage of energy down-conversion cascade is important for the production of quasiparticles and shown to split into two phases. The first is controlled by the evolution of the phonon distribution while the second is dominated by quasiparticle down-conversion. The relative duration of the two phases and hence the rates of quasiparticle generation depend on material parameters, and most common superconductors could be classified into three different groups. For typical superconductors used for x-ray detection the down-conversion cascade was shown to be fast compared to various time scales in the tunnelling regime.

Electro-deposited superconductor nanowires with controlled crystal texture

Ge Yi and Walther Schwarzacher
Department of Physics, Bristol University, Bristol, UK

Superconducting Pb wires (diameter 50 nm) with controlled crystal texture have been prepared by template electro-deposition. Pulsing the applied potential makes it possible to grow either polycrystalline or single-crystal wires selectively and reproducibly. Measurements of T_c reveal significant differences between the two types of nanowire.

Magnetoresistance and twiston scattering in carbon nanotubes

S.W.D. Bailey and C.J. Lambert
Physics Department, Lancaster, University, Lancaster LA1 4BY, UK

We investigate the electronic transport properties of armchair (conducting) Carbon Nanotubes. Firstly by way of the magnetoresistance with an axially applied magnetic field. Secondly, the effect of a small angular distortion produces a dramatic zero-bias suppression in the electrical conductance.

Superconducting quantum dots

Andrei Filip
Applied Physics Department, Groningen University of Technlogy,
Groningen, The Netherlands

We report on the recent development of technology of making superconducting quantum dots with various geometrical configuration.

Suppressed conductance oscillations in ferromagnetic Andreev interferometer

C.M. Newman
Physics Department, Lancaster University, Lancaster, LA1 4YB, UK

The large 2 probe conductance oscillations present in normal Andreev interferometers are suppressed if the normal metal is replaced by a ferromagnetic one, provided the distance between superconducting islands exceeds the Thouless length. Furthermore, in the ballistic case, as well as the diffusive case the amplitude of oscillation decreases as the exchange field increases and at intermediate values of the exchange field the zero-phase extremum can change from a maximum to a minimum.

Andreev reflection in strong magnetic fields

Ulrich Zuelicke
Inst. f. Theoret. Festkoerperphysik, Univ. Karlsruhe,
Engesserstr. 7, D-76128 Karlsruhe, Germany

We have studied the interplay of Andreev reflection and cyclotron motion of quasiparticles at a superconductor-normal-metal interface with a strong magnetic field applied parallel to the interface. Bound states are formed due to the confinement introduced both by the external magnetic field and the superconducting gap. These bound states are a coherent superposition of electron and hole edge excitations similar to those realized in finite quantum-Hall samples. We find the energy spectrum for these Andreev edge states and calculate transport properties.

Electron transport properties of F/S nanostructures

I. Sosnin, V. Petrashov, I. Cox, A. Parsons, C. Troadec
Holloway, University of London, Egham Surrey, TW20 0EX, UK

We report an experimental study of the superconducting proximity effect in hybrid ferromagnet/superconductor nanostructures. Developed phenomenological analysis accounts for many recent experimental results. Further experiments with different geometries and/or different materials are suggested.

Coulomb-repulsion-induced transport properties of N/S nanostructures

P. Dolby and C. J. Lambert
Physics Department, Lancaster University, Lancaster, LA1 4YB, UK

The change from an attractive to a repulsive interaction at a N-S interface causes a - shift in the order parameter phase. In the presence of tunnel barriers, this should have a pronounced effect on Andreev bound states. By solving the Bogoliubov - de Gennes equation in 2D, we illustrate this effect by computing the electrical conductance of a N-S contact both with and without such a phase shift.

Transport properties of Nb/InAs (2DEG) hybrid structures

Andreas Richter, Peter Erhart, Alexander Friedrichs, Toru Matsuyama, and Ulrich Merkt
Institut fur Angewandte Physik und Zentrum fur Mikrostrukturforschung,
Universitat Hamburg, Jungiusstr. 11, D-20355 Hamburg, Germany

We present electronic transport properties of superconductor/semiconductor hybrid structures formed by Nb electrodes in contact with the two-dimensional electron gas (2DEG) of high electron mobility InAs heterostructures. In recent experiments we focus on the direct observation of bound Andreev states.

Quasiparticles in High T$_c$ Superconductors

Z. Szotek[(a)], B. L. Gyorffy[(b)],W. M. Temmerman[(a)], O. K. Andersen[(c)], and O. Jepsen[(c)]
[(a)] *Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK*
[(b)] *H H Wills Physics Laboratory, University of Bristol,*
Tyndall Avenue, Bristol, BS8 1TL, UK
[(c)] *Max-Planck-Institut für Festkörperforschung,*
D-70506 Stuttgart, Germany

We present a semiphenomenological approach to calculating the quasiparticle spectra of High Temperature Superconductors (HTSC's). It is based on a particularly efficient parametrization of the effective electron-electron interaction afforded by the Density Functional Theory for superconductors and a Tight-Binding-Linearized-Muffin-Tin-Orbital scheme for solving the corresponding Kohn-Sham-Bogoliubov-de Gennes equations. We illustrate the method by investigating a number of site and orbital specific, but otherwise phenomenological models of pairing in quantitative detail. We compare our results for the anisotropy of the gap function on the Fermi surface with those deduced from photoemission experiments on single crystals of $YBa_2Cu_3O_7$. Also, we compare our results for the low temperature dependence of the specific heat with measurements. We investigate the doping dependence of the superconducting gap and transition temperature, T_c. We present new evidence that the Van Hove-like scenario is an essential feature of superconductivity in these materials. For the low temperature penetration depth our calculations at optimal doping are compared to measurements of A. Carrington *et al.*, revealing paramount importance of the chain in YBCO for zero temperature penetration depth. We observe a linear dependence of the low temperature penetration depth at all studied dopings. Since our description of pairing is semiphenomenological, we shed new light on the physical mechanism of pairing only indirectly and conclude, provisionally, that the dominant pairing interaction operates between electrons of opposite spin, on nearest neighbour Cu sites in $d_{x^2-y^2}$ orbitals.

7 General Workshop/Conference Announcements

7.1 A Euro-Workshop in Cambridge

COMPUTATIONAL QUANTUM MANY BODY PHYSICS

Organisers: P. B. Littlewood and P. Monthoux

18 - 21 February 2000

Advances in algorithms and computer hardware have opened many exciting avenues of research in quantum many-body physics. This Workshop will focus on methods for computational many body physics applied to strongly correlated electron systems.

Speakers already confirmed: W. Barford, E. Bickers, R. Bulla, D. Ceperley, T. Costi, D. Cox, S. Fahy, M. Foulkes, S. Fujimoto, O. Gunnarson, J. Inoue, R. Noack, A. Oles, W. Putikka, M. Rozenberg, R. Scalettar, S. Sorella, F. Tassone, W. Temmerman, M. Troyer, H. Tsunetsugu, P. Young.

Location: The Workshop will take place at the Newton Institute. Participants are expected to arrive on Thursday 17 February in the afternoon and the programme will be held from the morning of 18 February until the afternoon of 21 February. We will be able to accept a small number of additional applications and will be able to provide support for some EU researchers under 35 years of age.

Applications: Application forms are available from the WWW at:

http://www.newton.cam.ac.uk/programs/scew02.html

Completed application forms should be sent to Maureen Clark at the Newton Institute or via email to: m.clark@newton.cam.ac.uk.

This workshop is part of the six-month programme on Strongly Correlated Electron Systems at the Newton Institute being held from 5 January to 30 June 2000. For further details see:

http://www.newton.cam.ac.uk/programs/sce.html

Programme Contacts: P Monthoux (phm21@phy.cam.ac.uk)
P. Littlewood (pbl21@phy.cam.ac.uk)

7.2 DFT Conference in Antwerp

First Announcement of Conference on
Density Functional Theory and its Applications to Materials
University of Antwerp, Belgium
June 8 till 10, 2000

Organizing Committee:

V.E. Van Doren (Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen)
C. Van Alsenoy (Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk)
P. Geerlings (Faculty of Sciences, University of Brussels, Pleinlaan 2, 1050 Brussel)
E. Van Ocken (Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen)

Contributions

Applications are invited for the above International Conference. Any density functional studies relevant to materials science may be proposed, whether on three-dimensional materials (e.g. semiconductors and metallic alloys), or on low-dimensional systems (e.g. polymers or 2D electron gases in heterojunctions). Calculations on medium- or large-sized clusters will also be considered, if they clearly throw light on the understanding of bulk or surface properties of materials.

The following scientists have already accepted the invitation to lecture:

N.W. Ashcroft (*Cornell Center for Materials Science and Laboratory of Atomic and Solid State Physics, Cornell University, Clark Hall, Ithaca, NY 14853-2501, U.S.A.*)
G.B. Bachelet (*Dipartimento di Fisica, Universita di Roma, La Sapienza, Pl. AldoMoro 2, I-00185 Roma, Italy*)
A. Baldereschi (*Inst. Physique Applique, Ecole Polytechnique Fdrale, PHB Ecublens, CH-1015 Lausanne, Switzerland*)
R. Car (*Princeton University, Princeton, New Jersey 08544, U.S.A.*)
T.C. Collins (*Oklahoma State University, 203 Whitehurst Hall, Stillwater, OK 74078-0075, U.S.A.*)
J.T. Devreese (*Department of Physics, University of Antwerp, Universiteitsplein 1, B- 2610 Wilrijk, Belgium*)

R.W. Godby (*Department of Physics, University of York, , York YO10 5DD, U.K.*)
E.K.U. Gross (*Physikalisches Institut, Universitt Wurzburg am Hubland, D-97074 Wurzburg, Germany*)
O. Gunnarsson (*Max-Planck Institut, Postfach 800665, D-70506 Stuttgart, Germany*)
J. Krieger (*Physics Department, Brooklyn College of CUNY, 2900 Bedford Avenue, Brooklyn 11210, NY, U.S.A.*)
J. Ladik (*Lehrstuhl fr Theoretische Chemie, Universitt Erlangen, Eger landstrasse 3, D-91058 Erlangen, Germany*)
M. Levy (*Chemical Department, Tulane University, New Orleans, LA 70118, U.S.A.*)
S. Louie (*Department of Physics, University of California, Berkeley, CA 94720, U.S.A.*)
N.H. March (*presently at: Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen*)
J.L. Martins (*INESC, Rua Alves Redol 9, P-1000 Lisboa CODEX, Portugal*)
J. Mintmire (*Code 6189, Naval Research Laboratories, Washington, DC 20375-5342, U.S.A.*)
M. Payne (*Cavendish Laboratory, TCM-group, University of Cambridge, Madingley Road, Cambridge CB3 0HE, U.K.*)
F. Peeters (*Department of Physics, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium*)
J.P. Perdew (*Department of Physics, Tulane University, New Orleans, LA 70118, U.S.A.*)
G. Straub (*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.*)
D. Wallace (*T-1, MS B221, Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.*)

Persons whose applications are accepted will be encouraged to offer one hour poster presentations during the meeting.

All participants (maximum 150) are required to pay a registration fee of 250 EURO/$, which gives entitlement to conference documentation and proceedings, coffee and lunch, transportation to lecture hall and social program including a concert and the conference dinner.

For further information please contact:

V.E. Van Doren
Department of Physics
University of Antwerp
Groenenborgerlaan 171
B-2020 Antwerpen
Belgium
tel. +32/3/2180317
fax +32/3/2180318
e-mail: density@ruca.ua.ac.be

7.3 ESCM2000 Conference

Conference Announcement and Call for Papers
ESCM2000: Electronic Structure and Magnetism in Complex Materials
26-28 JULY, 2000
Washington, DC

We are pleased to announce the conference, ”ESCM2000: Electronic Structure and Magnetism in Complex Materials”, which will be held July 26-28, 2000 on the campus of Georgetown University. The goal of the conference is to bring together experts and students to discuss the electronic theory of magnetism and magnetic materials. Topic of particular interest include:

- Magnetic Semiconductors
- Magnetic Oxides
- Rare-Earth and Actinide Magnetism
- Half-Metals
- Molecular Magnets and Magnetic Clusters
- Non-Collinear Magnetism
- Magnetic Excitations
- Spin-Polarized Transport
- Spin Dynamics
- Strong Correlations and Magnetism
- Coupling Magnetic Scales: Atoms to Domains and Beyond

We hope to have substantial participation by young scientists, and to this end the costs for registration and housing will be very moderate, and additionally we expect to subsidize a number of the student attendees.

The format will allow plenty of time for discussion. It will consist of a small number of plenary talks by recognized experts in the field, invited talks that will be selected from the contributed abstracts and contributed (poster) sessions.

Details regarding registration and abstract submission are on the conference web site: http://cst-www.nrl.navy.mil/escm2000

We look forward to seeing you in Washington this summer.

7.4 Cagliari Workshop

The Physics Department, Universita' di Cagliari
and
Cagliari Research Unit of Istituto Nazionale per la Fisica della Materia
organize the

X WORKSHOP ON COMPUTATIONAL MATERIALS SCIENCE

7 - 12 September 2000
Tanka Village, Villasimius (CA), Sardinia, Italy

web page: http://www.dsf.unica.it/CMS2000
e-mail: workshop@dsf.unica.it

under the patronage of UNESCO

An international workshop on computational techniques and applications to materials science

See TENTATIVE INVITED SPEAKERS and INFO below.

FORMAT: About 20 invited lectures plus POSTER contributed session.

VENUE: Tanka Village at Villasimius (CA), an attractive sea resort on the south-eastern coast of Sardinia, providing comforts and an informal atmosphere.

CONTACT: For scientific and logistic queries: workshop@dsf.unica.it

CONTRIBUTIONS AND PROCEEDINGS:

Contributions in poster format are invited. ALL contributions will be published probably in a special issue of the journal Computational Materials Science. Deadline for abstract submission: July 31, 2000. Contact V. Fiorentini at +39 070 6754912 or P. Ruggerone at +39 070 6754847 or at workshop@dsf.unica.it for further details. Camera ready manuscripts will be due at the Workshop, LaTeX templates can be downloaded from the Workshop homepage: http://www.dsf.unica.it/CMS2000

INVITED SPEAKERS:

W. Kohn (UCSB, USA)	(DFT)
M. Parrinello (MPI-FKF, Germany)	(Car-Parrinello)
R. Resta (U Trieste, Italy)	(polarization theory)
A. Zunger (NREL, USA)	(semic. alloys and nanostructures)
M. Scheffler (FHI-MPG, Germany)	(surfaces and catalysis) (*)
U. Landman (Atlanta, USA)	(large-scale materials science simul.)
A. Baldereschi (EPFL, Switzerland)	(interfaces and contacts)
E. Tosatti (SISSA, Italy)	(high pressure physics) (*)
R. O. Jones (KFZ Juelich, Germany)	(polymers and clusters)
S. Baroni (SISSA, Italy)	(linear response and phonons)
M. Cardona (MPI-FKF, Germany)	(experiments: bulk) (*)
J. P. Toennies (MPI Goettingen, Germany)	(experiments: surfaces)

(*) not yet confirmed

REGISTRATION:

The REGISTRATION form can be sent directly from the Workshop homepage (http://www.dsf.unica.it/CMS2000). The deadline is July 1, 2000.

The registration should be accompanied by payment receipt of the CONFERENCE FEE (by FAX: ++39-070-510171). The fee includes full-board lodging at Hotel Tanka Village from 7/9 afternoon to 12/9 lunch, coffee breaks, refreshments, social trip (or banquet), and amounts to:

Double room lodging It.Lire 900000 (∼ US $ 470)/person Single room lodging It.Lire 1000000 (∼ US $ 520)/person.

PAYMENT should be effected by bank money transfer on the bank account number 22698 of Comitato Organizzatore di Attivita' di Fisica Computazionale, at Banco di Sardegna, Sede di Cagliari, Codice ABI 1015/7 - CAB 04800.

No fee is requested from the invited speakers.

The Organizing Committee hopes to be able to offer partial support to a limited number of young scientists, preferrably PhD students. Since this possibility depends on funds availability, support will be decided upon shortly before the workshop.

Series Chairman : prof. A. Baldereschi - EPFL Lausanne Workshop Chairman : prof. F. Meloni - INFM and Universita‘ di Cagliari Scientific Secretariat: dr. V. Fiorentini - dr. P. Ruggerone INFM and Universita‘ di Cagliari.

7.5 Symposium on Spin-Electronics

Please note the above conference will take place on

3-6 July 2000 in Halle, Germany.

Detailed information about program, abstract submission (deadline February 29, 2000), registration, etc., is available from the conference web site:

http://www.mpi-halle.de/ sse2000/

P. Bruno

7.6 ChiPPS Workshop

2nd International Workshop on Challenges in Predictive Process Simulation
Wandlitz, Germany, 15-18 May 2000
ChiPPS'2000
http://www.ihp-ffo.de/chipps/00/Welcome.html
SECOND ANNOUNCEMENT AND CALL FOR ABSTRACTS

ChiPPS is a series of interdisciplinary meetings aimed to bring together experts from three distinct fields:

- fundamental materials science,
- development of process simulation tools,
- manufacture of microelectronic devices.

In particular, it serves as a bridge between those who study physical properties at the atomic scale and those who simulate technological processing steps at the macroscopic level.

The purpose of ChiPPS is to identify current and anticipated challenges in process simulation for microchip technology from the point of view of technologists, programmers, and physicists. It is a "call for action" meeting, meant to stimulate a new wave of research relevant to process simulation by clarifying the needs and pointing out advantages and deficiencies in the existing theoretical and experimental approaches. A review paper summarizing ChiPPS'97 can be downloaded from:
http://www.ihp-ffo.de/chipps/97/Ddoc/dpg.html

ChiPPS'2000 will be held in Wandlitz near Berlin, Germany, from 15 to 18 May 2000. Papers are solicited on subjects covering semiconductor physics and technology, such as:

- Diffusion in solids;
- Carrier transport in nanostructures;
- Deposition of dielectrics and metals;
- Epitaxial growth of semiconductors;
- Formation of silicide films;
- Reliability of dielectrics and interconnects;
- New materials for microelectronics;
- New concepts for microelectronic devices.

To receive full consideration, abstracts of contributed papers should be submitted before the deadline of 1 February 2000.

For more details, please see the Call for Papers posted at:
http://www.ihp-ffo.de/chipps/00/Welcome.html

The invited presentations include:

U. Schwalke, Infineon, CMOS for Everyone
R. Stumpf, Motorola, DFT for Everyone
P. Vogl, Muenchen, Physics for Process and Device Simulation
A. Jelenski, IEMT, Compound Semiconductors: a Growing Market
W. Choyke, Pittsburgh, SiC technologies
W. Schoenmaker, IMEC, Modeling of Electromigration in Interconnects
A. Sutton, Oxford, Kinetics of Diffusional Phase Transitions
K. Maex, IMEC, Silicides and Metals
O. Nalamasu, Bell Labs, Lithography for Deep Submicron CMOS
R. Singh, Clemson, Alternative Dielectrics
A. Korkin, Motorola, Atomistic Modeling of CVD
W. D. Rau, IHP, 2D Imaging of Dopant Profiles
H.-J. Osten, IHP, SiGeC for Wireless Communication
M. Tomozawa, Troy, Mechanisms of Chemical Mechanical Polishing
M. J. Caldas, Sao Paulo, Segregation of Dopants to Interfaces
S. Cristoloveanu, Grenoble, Silicon-On-Insulator Technologies
A. Aviram, IBM, Do We Need Molecular Computers
H.-J. Gossmann, Bell Labs, Atomistic Physics for Microelectronics

For a full list of lectures see the scientific program at:
http://www.ihp-ffo.de/chipps/00/

Dr. Jarek Dabrowski
Institute for Semiconductor Physics
P.O. Box 1466
D-15204 Frankfurt(Oder)
Germany
Tel.: +49(335)5625-316
Fax: +49(335)5625-300
E-mail: jarek@ihp-ffo.de

E-mail with subject "ChiPPS inform" to receive regular posting
E-mail with subject "ChiPPS remove" to receive no more posting

7.7 Applied DFT2001 Conference

Conference on

Applied Density Functional Theory

January 14-17, 2001

Vienna, Austria

http://www.physics.at/dft2001

dedicated to Karlheinz Schwarz
on occasion of his 60th birthday

Honorary Chairman: Walter Kohn

The Conference

This four day symposium will focus on the application of Density Functional Theory to problems in physics, chemistry and materials science. It is dedicated to Karlheinz Schwarz on occasion of his 60th birthday.

Venue

The conference will take place at the Vienna University of Technology, Vienna, Austria, conveniently located in the city center. Scientific Program The scientific program will include invited talks, oral presentations and posters. Invited speakers confirmed so far include:

Ole Andersen, Stuttgart, Germany
Peter Blchl, Zrich, Switzerland
Roberto Car, Princeton, USA
Brje Johansson, Uppsala, Sweden
Walter Kohn, Santa Barbara, USA
Dimitrios Papaconstantopoulos, Washington,USA
David Singh, Washington, USA
Erich Wimmer, Paris, France

Conference Book

Extended abstracts will be published.

Conference Fee

The conference fee includes receptions, coffee breaks and the conference dinner. It is estimated to be 220 EURO for participants and 150 EURO for students.

Registration

Pre-registration, final registration and abstract submission are possible online on the conference web site.

Pre-registration

We would appreciate if you make use of this service. The second circular will only be sent to those who have pre-registered.

Preliminary Schedule

Participants are expected to arrive by Sunday, January 14. On Sunday evening a welcome reception will be held. The conference dinner will take place on Tuesday and the conference will end on Wednesday evening.

Deadlines

June 2000 second circular will be mailed to those who have pre-registered September 30, 2000 deadline for abstract submission and payment of the early registration fee

Organizing Committee

Claudia Ambrosch-Draxl, Graz, Austria
Peter Blaha, Vienna, Austria
Ccile Hbert, Vienna, Austria
Joachim Luitz, Vienna, Austria
Matthias Scheffler, Berlin, Germany
Jorge Sofo, Bariloche, Argentina

Contact

Web: http://www.physics.at/dft2001

Mail: dft2001@physics.at

Phone: +43-1-58801-15679 (Joachim Luitz)

Fax: +43-2231-67443

Postal Address: Applied DFT2001
c/o Joachim Luitz
Inst. f. Phys. Chem.
TU Wien
Getreidemarkt 9/156
A-1060 Vienna
AUSTRIA

With Density Functional Theory into the 3rd Millenium ...

8 General Job Announcements

Postdoctoral/Research Associate Positions in Electronic Structure Theory

National Renewable Energy Laboratory (NREL)
http://www.sst.nrel.gov

NREL's Solid State Theory Group is looking to fill two postdoctoral/research associate positions in the area of Electronic Structure Theory. These positions would be working with Dr. Alex Zunger and are for 2-3 years. The first position is in a new exciting project on theory of doping and doping bottlenecks in semiconductors and insulators and is available immediately, so apply now. The second position is in the area of alloy electronic structure theory, to start summer or fall 2000; applications for this position will be accepted for one month after publication of this ad. Applicants are expected to have a background in solid-state theory. Depending on experience and qualifications, either positions could be at the rank of post-doctoral fellow ($40,000-$47,000 per year) or Research Associate ($52,000-$65,000 per year). More details about ongoing work in the group, computer facilities, personnel, publications are included in http://www.sst.nrel.gov. Clarification or further details can be obtained via e-mail to azunger@nrel.gov.

Interested candidates should send immediately a curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two references addressed to:

Dr. Alex Zunger
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401, USA

NREL is an equal opportunity employer and proud of its commitment to diversity. Women and minorities are encouraged to apply.

Post-Doc Position
Condensed Matter Theory Sector
International School for Advanced Studies in Trieste (Italy)

A postdoctoral position is available, starting immediately, for 1 year on a on a project entitled:

"Density-functional theory-based molecular dynamics of biological systems"

The work will involve applications of the Car-Parrinello to systems of pharmaceutical relevance, such as targets for anti-AIDS and anti-cancer therapy.

Candidates should hold a Ph.D in Physics or Chemistry or have equivalent research experience and have good computing and physical modeling skills.

Further information can be obtained from Dr. Paolo Carloni, International School for Advanced Studies, SISSA, via Beirut 4, 34014 Trieste, Italy

http://www.sissa.it/cm/bc/

email: carloni@sissa.it

Phone: +39-040-3787407, Fax:+39-040-3787528

Announcing a Grant for Graduate Studies in Physics

University of Valladolid (Spain)

The research Project ”Nanotubes and Other nanostructures of technological interest” (ref. PB98-0345) is sponsored by the DGES (Direccion General de Enseanza Superior) of Spain. That Project will be carried out in the University of Valladolid (Spain) in the group of Professor Julio A. Alonso (Departamento de Fsica Terica).

Most likely this Project will be awarded a Grant allowing a graduate student to work in a Ph D Thesis Project in this Department. The research work will focuss on the theoretical study of the electronic structure of atomic clusters and nanostructures, in particular fullerenes and carbon nanotubes, and in the computational simulation of their physical and chemical properties.

We invite interested young citicens of any country of the European Union, having completed a B. S. Degree in Physics or Chemistry to send the application to:

Professor J. A. Alonso
Departamento de Fsica Terica
Universidad de Valladolid
47011 Valladolid, Spain

The material that has to be submitted includes:

1. Application. The application forms can be obtained from Ministerio de Educacion y Cultura of Spain in the following internet address:
   http://www.seui.mec.es
2. Curriculum Vitae
3. Photocopy of the passport or equivalent identification
4. An official Academic certificate of having completed the undergraduate studies, with full details of the courses attended and the grades obtained.
5. Two reference letters (optional)

For further information, contact Prof. J. A. Alonso (email: jaalonso@fta.uva.es, phone: 34-983-423142, fax: 34-983-423013)

POST-DOCTORAL POSITIONS
SISSA/ISAS TRIESTE

The International School for Advanced Studies (SISSA/ISAS) in Trieste expects to offer 4 post-doctoral positions in the field of

Theory of Condensed Matter.

These positions will be available from the Fall of 2000 for one year and renewable for a second year. Candidates, who must not be over 36 years of age, should submit immediately their applications with their Curriculum Vitae, list of papers and preprints, and a tentative non committal research programme. They should arrange for at least two letters of reference and any other useful information to be sent by the same date. Email applications are welcome, but a hardcopy should also reach the School anyway before the deadline.

Applications and correspondence should be sent to:

Postdoc Programme
International School for Advanced Studies
Via Beirut, 2-4
34014 TRIESTE - ITALY
email: postdoc@sissa.it
fax (+39) 40 3787528

NANOPHASE Research Training Network

Seven Postdoctoral Positions and a PhD Studentship in the Theory of Nanoscale Structures

NANOPHASE (nanoscale photon absorption and spectroscopy with electrons) is a new Research Training Network, approved for funding (subject to contract) by the European Union. The overall topic of the Network is the theory of nanometre-scale structures - atomic clusters, quantum dots on surfaces or embedded in materials, quantum wires, and molecules adsorbed on surfaces - and the spectroscopic processes that can be used to characterise those structures, their electronic and optical properties, and their growth. These will be studied using fundamental theory and state-of-the-art ab initio computer simulations. The seven NANOPHASE teams (Fritz Haber Institute, Berlin; Friedrich Schiller University, Jena; Lund University; CNRS / Ecole Polytechnique, Paris; University of Rome ”Tor Vergata”; University of Valladolid; University of York) expect to have seven postdoctoral positions and one PhD studentship available shortly, to start in mid-2000.

Availability of these Network-funded vacancies is subject to the final completion of the Network contract with the European Commission, expected to be confirmed in February 2000. To be eligible for an Network-funded appointment the applicant must satisfy the EU's criteria which are, in brief:

- aged 35 years or less (with certain exceptions)
- a citizen of a member state of the European Union or a state associated with the Fifth Framework Programme
- resident and working outside the proposed host country for more than 12 months of the last two years.

Details of the positions and how to apply are given on the Network's web page, http://www-users.york.ac.uk/ rwg3/nanophase.html.

POSTDOCTORAL POSITION

Department of Theoretical Condensed Matter Physics
Universidad Autonoma de Madrid
Madrid, Spain

A postdoctoral position at the Department of Theoretical Condensed Matter Physics of the Universidad Autonoma de Madrid (Spain) is available, starting between March and September 2000. The position is funded by the European Research and Training Network ”Designing Inorganic/Organic Devices” and the project will be supervised by Prof. F. Flores. Only citizens of the European Union or associated states (excluding Spain) are eligible. The position is for one year, with the possibility of renewal for up to three and a half years upon mutual agreement.

The research will be addressed to understanding the electronic properties of interfaces formed with organic thin films deposited on inorganic semiconductors. A typical example is the organic molecule PTCDA, and the corresponding interface to be analyzed is GaAs/PTCDA/metal, where the semiconductor is a GaAs(100)-saturated surface. In this research, different LDA codes and tight-binding methods will be used to characterize the organic molecule and the interface. Many-body effects associated with the electronic properties of the organic molecule can be expected to introduce new effects at the interface formation. The research will be performed in close collaboration with the other theoretical and experimental groups of the Network.

Candidates should have a PhD in Physics or Chemistry, and be interested in microscopic simulations. Preference will be given to candidates with experience in calculations of electronic properties of materials using LDA and tight-binding codes.

Interested candidates should send his/her CV and two letters of reference to:

Prof. F. Flores
Departamento de Fisica Teorica de la Materia Condensada
Universidad Autonoma de Madrid
E-28049 Madrid, Spain

FAX: +34-91-3974950
email: fernando@uamc14.fmc.uam.es

POSTDOCTORAL POSITION
Electronic Structure Group
Department of Physics
Case Western Reserve University, Cleveland, Ohio, U.S.A.

A postdoctoral position is available immediately in the group of **Walter Lambrecht**. The candidate should have a Ph. D. and experience in electronic structure calculations. Current research topics are electronic structure of defects in semiconductors and studies of nonlinear optical materials and properties. The position is initially for one year but renewable up to 3 years. For further information, see contact information below. Send CV, including a description of your research interests and experience, and names of at least two references to:

Prof. Walter R. L. Lambrecht
Department of Physics
Case Western Reserve University
10900 Euclid Avenue
Cleveland, OH 44106-7079, U.S.A.

or, preferably, by email to:
walter@els.phys.cwru.edu
phone: (216) 368-6120
fax: (216) 368-4671

POSTDOCTORAL POSITION
Fritz Haber Institute of the Max Planck Society
Berlin, Germany

A postdoctoral position at the Fritz-Haber-Institut in Berlin (Germany) is available, starting March 2000. The position is funded by the European Research Training Network "Interface analysis at atomic level and Properties of Advanced Materials (IPAM)". Only citizens from the European Union (excluding Germany) or associated states are eligible for this position. The position is for one year, with the possibility of renewal for up to three years upon mutual agreement. The study will be performed in the group "Surface morphology and growth of semiconductors" under the supervision of Dr. Joerg Neugebauer.

The research will be mainly focused on the theoretical modeling of electronic properties and atomic structure of interfaces and interfacial defects employing first principles total energy calculations. The basic materials for this project will be gallium nitride based semiconducting layers where extended defects are well known to occur in large concentrations. The research will be performed in close collaboration with experimental, industrial, and theoretical partners within the EC. Strong interaction with the other groups is therefore expected.

The successful candidate should have a PhD in Physics, Chemistry or Materials Science, and have a strong interest on microscopic simulations. Preference will be given to candidates with strong background in any (or several) of these fields: electronic structure calculations, molecular modeling, density functional theory, empirical potentials, and analysis of transmission electron microscopy measurements.

Interested candidates should send immediately a CV, list of publications, and name and address (including email) of three references, preferably by email or fax, to:

Dr. Joerg Neugebauer
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4-6
D-14195 Berlin-Dahlem
Germany

WWW: http://www.fhi-berlin.mpg.de/th/JG
E-mail: neugebauer@fhi-berlin.mpg.de
Phone: ++49 30 8413 4826
FAX: ++49 30 8413 4701

POSTDOCTORAL POSITION

Department of Physics, University of Cambridge, UK

A postdoctoral position is available from 1st October 2000 to work on quantum Monte Carlo calculations with Dr Richard Needs. We use variational and fixed-node diffusion quantum Monte Carlo methods to study problems in condensed matter physics. More information on the work of the group can be found at:

http://www.tcm.phy.cam.ac.uk/ rn11/

The successful candidate should have a PhD in Physics, Chemistry, Materials Science or a related subject. Preference will be given to candidates with a strong background in electronic structure calculations, but experience with quantum Monte Carlo methods, although advantageous, is not necessary.

Details of how to apply can be found at:

http://www.tcm.phy.cam.ac.uk/advert.html

Richard Needs,
TCM Group, Cavendish Laboratory,
Madingley Road,
Cambridge CB3 0HE,
UK
E-mail: rn11@phy.cam.ac.uk

PH.D. STUDENTSHIP
Institute of Materials Science (ICMAB-CSIC)
and
National Center for Microelectronics (CNM-CSIC)
Barcelona, Spain

A PhD student position is available under the framework of the ATOMCAD network financed by the EU, to be executed in the next three years. Only nationals of Member or Associate States of EU (excluding Spain) are eligible for the position. Candidates should have a good background on condensed matter physics and computing experience. They should also be able to work in closed collaboration with electrical engineers and experimental physicist. The study will be performed jointly at the Materials Research (ICMAB) and Microelectronics (CNM) Institutes of the CSIC in Barcelona under the supervision of Dr. Pablo Ordejon and Dr. Jose Rebollo.

The research will be directed towards understanding the mechanisms of damage formation and its recovery, as well as the activation of dopants in silicon carbide (SiC) during ion implantation processes for semiconductor device fabrication. The specific activities include: (1) Modeling of the implantation processes (depth distribution of implanted ions and lattice damage) by a Monte Carlo simulator based on the binary collision approximation (BCA) developed in our group. (2) Improve the BCA modeling using data from specifically designed experiments, including random and aligned implantations. (3) Investigate the nature and distribution of primary defects (vacancies, interstitials, etc.) using classical and quantum-mechanical molecular dynamics simulations, and understand the evolution of defects for damage build-up. (4) Perform first-principles calculations of electronic states at the dopants and defect sites to understand the mechanism of defect annealing and dopant activation.

Persons interested should send their resume to:

Dr. Pablo Ordejon
Instituto de Ciencias de Materiales de Barcelona (ICMAB-CSIC)
Campus de la UAB, 08193 Bellaterra
Barcelona, Spain
E-mail: ordejon@icmab.es

or to:

Dr. Jose Rebollo
Instituto de Microelectronica de Barcelona
Centro Nacional de Microelectronica (CNM-CSIC)
Campus de la UAB, 08193 Bellaterra
Barcelona, Spain
E-mail: rebollo@cnm.es

At Uppsala University in the charming beautiful Sweden there are available

Two PhD-studentships in Condensed Matter Theory

1. Combined theoretical and experimental STM studies

   This project combines first principles theoretical calculations and scanning tunnelling microscopy (STM) experiments to achieve a better understanding of STM as an experimental tool and to provide the experimental basis that theory needs. Two fields of interest are proposed: first to study general trends in formation of III-V semiconductor surfaces, second to study surface magnetism and small magnetic structures on the atomic level. We will develop spin-resolved STM, both experimentally and theoretically, to make it a useful universal tool.

2. Magnetoelectronics: First-principles studies of Ferromagnet/Semiconductor Interfaces

   In the rapid growing field of magnetoelectronics, hybrid structures of ferromagnets and semiconductors play an essential role. Therefore the detailed knowledge of the ferromagnet/semiconductor interface properties is of high priority. The tools in this project are first principles local-density-functional total-energy calculations. The issues to be addressed include interlayer exchange coupling, alloying, interface intermixing, reconstruction, Schottky barrier, and the influence of defects on the interface properties.

We offer outstanding computational facilities and an inspiring research atmosphere. Your salary will make life in Sweden enjoyable. Contact us for more details!

More information about our research group in general may be found at http://www.fysik4.fysik.uu.se/

Interested candidates should contact us as soon as possible:

Dr Susanne Mirbt (E-mail: susanne.mirbt@fysik.uu.se)
Professor Brje Johansson (E-mail: borje.johansson@fysik.uu.se)
Uppsala University
Condensed Matter Theory
Box 530
S-75121 Uppsala
Sweden

Postdoctoral Position

Uppsala University, Sweden

Electronic Structure Calculations of Defect Properties at Semiconductor Heterointerfaces

A post-doctoral position is available in the Condensed Matter Theory group (Prof. Brje Johansson) at Uppsala University in Sweden.

The research will be mainly focused on the understanding of semiconductor laser degradation, i.e. the understanding of defect migration and defect accumulation at semiconductor heterointerfaces, using density functional methods. This project is part of a collaboration with the ERICSSON corporation.

We offer outstanding computational facilities and an inspiring research atmosphere. The position is available for up to two years. The salary amounts up to 20000 SKr/month (taxfree) depending on qualification.

More information about our research group in general may be found at http://www.fysik4.fysik.uu.se/

Interested canditates should send as soon as possible a CV, publication list, and references to:

Dr Susanne Mirbt
Condensed Matter Theory
Box 530
S-75121 Uppsala
Sweden
susanne.mirbt@fysik.uu.se

URGENT ANNOUNCEMENT

2 POST-DOCTORAL POSITIONS (*)

Departamento de Fisica Teorica, Atomica y Molecular, Universidad de Valladolid, Valladolid, Spain

The positions are available next year and are for two years, with possibility of extension. Further information on the research of our group as well as a publication list can be found in our web page:
http://www.fam.cie.uva.es/ arubio.

Applications should include a curriculum vitae, highlighting the main contributions, and a complete list of publications with an indication of those which the applicant selects as the most relevant for the application. reference letters will be given proper consideration. Accepted formats are paper, ascii/LaTeX/postscript/pdf email attachment, or a web address for html, LaTeX, ps, or pdf versions of the above. xxx or PR-online links are ok for the publication. Web links are the preferred format for all materials Applications should be sent to Dr. Angel Rubio (see below).

NOTE: The applicant must comply with the RTN rules for network employment of young scientists: The applicant should hold a Ph.D. degree or equivalent in Physics, Chemistry or Materials Science, be younger than 35, and should have some experience in computational Condensed Matter Theory. Preference will be given to candidates with strong background in any (or several) of these fields: electronic structure, molecular dynamics and transport calculations in nanostructiures and bulk systems, optical properties of materials, many-body interactions, and time-dependent density-functional-theory.

(*) 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 (excluding Spain) and states from the former Easter countries are eligible for the position, allocated to the Valladolid (Spain) node.

A) Postdoctoral position to work on Nanotubes

Candidates are invited to apply for a post-doctoral position to work on the growth mechanism, electronic, optical, structural and transport properties of carbon and composite-nanotubes with particular emphasis on theoretical calculations of interest for: STM microsopy, nanodevices, chemical activity, mechanical behavior, optical response. In addition, the group is flexible and open to promising new research directions within the general topic of nanotubes. The techniques to be used range from semiempirical potentials to acurate ab-initio methods. Knowledge of molecular dynamics and electronic structure calculations is desirable.

The project is included in a new EU-funded project continuation of a previous Training and Mobility Research TMR) Network on "Nanotubes for Microstructure Technology . A very close collaboration with the experimental partners of the network (groups in France, Germany, Belgium and Ireland) is guaranteed.

The objetives of the new program are:

i) To have a clear and consistent understanding og the growth mechanism of nanotubes.

ii) Development of composited systems

iii) The understanding and control of the correlation between mechanical (bending, torsion, extension, contraction, etc..)and electronic properties (electronic structure, electrical conductivity, Hall effect, magnetoresistance) of single-wall nanotubes.

iv) Technological applications.

B) Postdoctoral position to work on Electronic Excitations in Nanoscale Materials

The project is included in an EU-funded Network on "Nanoscale photon absorption and spectroscopy with electrons " (NANOPHASE). A very close collaboration with the theoretical partners of the network (groups in U.K, France, Italy, Germany and Sweden) is guaranteed. Please see the web page of the Network for further details (NANOPHASE).

The overall topic of the Network is the science of nanometre-scale structures - atomic clusters, quantum dots on surfaces or embedded in materials, quantum wires, and molecules adsorbed on surfaces - and the spectroscopic processes that can be used to characterise those structures, their electronic and optical properties, and their growth. Nanostructures are expected to underlie much of future technology, based in most cases on their optical and electronic properties. Our aim is to produce a detailed description and understanding of these properties, together with state-of-the-art computer simulation software. The Network's four key objectives are: -To achieve a detailed understanding of the relation between the structural properties, the optical absorption spectrum and the spectral function of quantum dots and clusters of semiconductor and metal atoms of up to 100 or more atoms, both isolated and embedded in bulk materials, together with general ab initio computer programs (not requiring the use of adjustable parameters).

-To calculate and analyse the optical absorption spectrum, the spectral function, and the electronic quantum conduction properties of one-dimensional nanostructures such as nanometre-scale metal wires and hollow tubes.

-To achieve a detailed understanding of the optical absorption and reflection spectra, the electron energy loss spectrum, the single-particle spectral function and the excited-state potential energy functions for molecular ad-/desorption, of a variety of surfaces important for nanometre-scale growth processes.

Applications should be sent to:

Dr. Angel Rubio
Departamento Fisica Teorica
Universidad de Valladolid
E-47011 Valladolid. SPAIN
Phone : ++34-983-423263
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http://www.fam.cie.uva.es/ arubio

Postdoc Positions at Rutgers University

One or more postdoc positions may become available beginning summer or fall 2000, associated with Profs. David Langreth, Karin Rabe, and David Vanderbilt in the computational materials theory group, Department of Physics and Astronomy, Rutgers University. Experience with density-functional-based methods is strongly advantageous.

Interested applicants should arrange for a CV and three letters of recommendation to be sent to Prof. Vanderbilt:

Prof. David Vanderbilt
Dept. of Physics and Astronomy
Rutgers University
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USA
E-mail: dhv@physics.rutgers.edu

9 Abstracts

Ab-initio molecular dynamics with a classical pressure reservoir: simulation of pressure-induced amorphization in a $Si_{35}H_{36}$ cluster

R. Martoňák[1], C. Molteni[2] and M. Parrinello
Max Planck Institut für Festkörperforshung
Heisenbergstrasse 1, D-70569 Stuttgart (Germany)

Abstract

We present a new constant-pressure ab-initio molecular dynamics method, suitable, e.g., for studying pressure-induced structural transformations in finite non-periodic systems such as clusters. We immerse an ab-initio treated cluster in a model classical liquid, described by a soft-sphere potential, which acts as a pressure reservoir. The pressure is varied by tuning the parameter of the liquid potential. We apply the method to a $Si_{35}H_{36}$ cluster, which undergoes a pressure-induced amorphization at $\sim$ 35 GPa, and remains in a disordered state even upon pressure release.

(Phys. Rev. Lett. in press)
Preprints available from: martonak@prr.mpi-stuttgart.mpg.de

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[2] Theory of Condensed Matter group, Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, Great Britain

Screened Real-Space Korringa-Kohn-Rostoker description of the relativistic and magnetic properties of transition metals

L. Petit[1,2], S.V. Beiden[1], W.M. Temmerman[3], Z. Szotek[3], G.M. Stocks[4]
and G.A. Gehring[1]
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Sheffield S3 7RH, UK
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Abstract

The use of the relativistic and spin-polarized real-space Korringa-Kohn-Rostoker (KKR) method is limited to small systems (less than 100 atoms). This is due to the prohibitively large CPU-times needed for the inversion of the KKR-matrix. To study systems of more than a thousand atoms, we have implemented the concept of a screened reference medium, within the fully relativistic spin-polarized version of the real-space locally self-consistent multiple scattering method (LSMS). The LSMS method makes use of a local interaction zone (LIZ) for solving the quantum mechanical problem, while the Poisson equation is solved in the whole space. The screened reference medium gives rise to sparse KKR-matrices and substantial reduction in the CPU-times, enabling applications of the method to systems whose LIZ consists of more than a thousand atoms. The method is benchmarked by application to the elemental transition metals, the fcc (face-centered-cubic) Co and Ni, and the bcc (body-centered cubic) Fe, and compared to the results of the conventional $\mathbf{k}-$space methods. The convergence in real-space of the magnetic moments, the magnetocrystalline anisotropy energy and orbital moment anisotropy is discussed in detail.

(Submitted to Phys. Rev. B)
Manuscripts available from: W.M.Temmerman@dl.ac.uk

Contesting results for magnetic moments in nickel thin films

A. Ernst, G. van der Laan, W. M. Temmerman, S. S. Dhesi and Z. Szotek
Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom

Abstract

We report on Korringa-Kohn-Rostoker Green's function calculations for the ground state moments of ultra thin Ni films on Cu(001) and on 4 monolayers (ML) Co/Cu(001). The calculations for Ni/Cu(001) show a slight enhancement of the Ni magnetic moment at the surface but a large reduction of the Ni magnetic moment at the Cu interface. The number of *d* holes at the surface and interface shows a small enhancement. The absence of a Cu magnetic moment appears to be the reason of this strong reduction in the Ni interface magnetism. However, for Co/Cu(100) the calculation gave a slightly increased interface magnetic moment. For Ni on a ferromagnetic substrate, such as 4 ML Co/Cu(001), this reduction does not occur, so that Ni at the interface retains its bulk value. These results are in contradiction with recent experimental results obtained using x-ray magnetic circular dichroism on ferromagnetic Ni films grown epitaxially on ultrathin films of Co. For decreasing film thickness, the number of holes and the magnetic moment show a gradual decrease.

(Submitted to Phys. Rev. B)
Manuscripts available from: W.M.Temmerman@dl.ac.uk

Defect structures on epitaxial $Fe_3O_4(111)$ films

Sh. K. Shaikhutdinov, M. Ritter, X.-G. Wang, H. Over, and W. Weiss
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6,
14195 Berlin-Dahlem, Germany

Abstract

Epitaxial $Fe_3O_4(111)$ films were grown onto a Pt(111) substrate by repeated cycles of iron deposition and subsequent oxidation in 10^{-6} mbar oxygen. A previous low energy electron diffraction (LEED) intensity analysis revealed the regular $Fe_3O_4(111)$ surface to expose 1/4 monolayer Fe atoms over a close-packed oxygen layer underneath. With scanning tunnelling microscopy (STM) a hexagonal lattice of protrusions with a 6 Å periodicity is observed. The protrusions are assigned to the topmost layer Fe atoms, which agrees with the dominating Fe 3*d* electron density of states near the Fermi level related to these surface atoms, as revealed by *ab initio* spin-density-functional theory calculations. The most abundant type of point defects observed by STM are attributed to iron vacancies in the topmost layer, which was confirmed by LEED intensity calculations where different types of vacancy defects have been simulated. For oxidation temperatures around 870 K the regular $Fe_3O_4(111)$ surface coexists with several different surface structures covering about 5 of the films, which expose 3/4 ML iron atoms or close-packed iron and oxygen layers, resulting in surface domains that are FeO(111) and $Fe_3O_4(111)$ in nature. These domains are arranged periodically on the surface and form ordered biphase superstructures. At 1000 K oxidation temperature they vanish and only the regular $Fe_3O_4(111)$ surface remains.

Phys. Rev. B **60**, 11062–11069 (1999)
Contact person: W. Weiss (weiss_w@fhi-berlin.mpg.de)

The effect of the environment on α-Al_2O_3 (0001) surface structures

X.-G. Wang, A. Chaka, and M. Scheffler
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14195 Berlin-Dahlem, Germany

Abstract

We report that calculating the Gibbs free energy of the α-Al_2O_3 (0001) surfaces in equilibrium with a realistic environment containing both oxygen and hydrogen species is essential for obtaining theoretical predictions consistent with experimental observations. Using density-functional theory we find that even under conditions of high oxygen partial pressure, the metal terminated surface is surprisingly stable. An oxygen terminated α-Al_2O_3 (0001) surface becomes stable only if hydrogen is present on the surface. In addition, including hydrogen on the surface resolves discrepancies between previous theoretical work and experimental results with respect to the magnitude and direction of surface relaxations.

Phys. Rev. Lett. (to be published)
Contact person: Anne Chaka (chaka@fhi-berlin.mpg.de)

An excited state density functional theory study of the rhodopsin chromophore

C. Molteni, I. Frank and M. Parrinello
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Heisenbergstrasse 1, D-70569 Stuttgart (Germany)

Abstract

Using a recently developed scheme for performing, within density functional theory, molecular dynamics and geometry optimisation for fairly large systems in the first excited singlet state, we have studied the structure and energy changes that the rhodopsin chromophore undergoes during the photoisomerisation from *11-cis* to *all-trans*. We discuss the effects of relevant parts of the protein environment close to the chromophore on the isomerisation barrier and on the chromophore structure.

J. Am. Chem. Soc. **121**, 12177 (1999)
Reprints available from: cm10020@phy.cam.ac.uk

Phase Diagram of Tetragonal Manganites

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Abstract

Phase diagram of $La_{1-x}Sr_xMnO_3$ as a function of hole doping x and tetragonal distortion c/a, which consists of ferromagnetic (FM), A-, C- and G-type antiferromagnetic (AF) states, is obtained by the first-principles band structure calculations. Effects of tetragonal distortion on the magnetic ordering are discussed in terms of orbital ordering and anisotropy in the hopping integrals. The general sequence of the magnetic ground states, FM → A-AF → C-AF → G-AF with the increase of x, is also explained based on the instability of FM states with respect to the spin-wave excitations.

(Accepted in Phys. Rev. Lett.)
Copy available from: zfang@jrcat.or.jp

Interface magnetism and electron redistribution

S. S. Dhesi, H. A. Dürr, E. Dudzik, and G. van der Laan
Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK
N. B. Brookes
European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

Abstract

The electronic structure at the Ni/Co interface has been characterised using differences in $L_{2,3}$ x-ray absorption spectra (XAS) recorded before and after deposition of Ni overlayers on Co films. Strong changes in the Co and Ni absorption spectra suggest a high degree of d charge redistribution between the Co and Ni d states for submonolayer coverages of Ni. X-ray magnetic circular dichroism shows that the change in the d state occupancies results in an increased Co spin moment and a reduced Ni spin moment. The effects are interpretted in terms of a modified exchange splitting of the Ni and Co d bands determined using line shape analysis of Co XAS. The results are compared with the predictions of first-principles band-structure calculations invoking the local spin-density approximation.

(Accepted for Phys. Rev. B)
Preprints available from: g.vanderlaan@dl.ac.uk

Canted Spin Ordering in Three-Dimensional Perovskite Manganites

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and
Tsukuba Advanced Computing Center,
1-1-4 Higashi, Tsukuba, Ibaraki 305-8561, Japan

Abstract

We reexamine the double-exchange picture of the canted spin arrangement in three-dimensional perovskite manganites $R_{1-x}D_x\mathrm{MnO}_3$ (R= trivalent rare-earth ion, D= divalent ion) proposed by de Gennes about forty years ago. Our approach is based on the multiple-scattering formalism, takes into account the double degeneracy of e_g orbitals, and allows to address the problem of the local stability of the canted spin states with respect to other more complicated forms of the noncollinear spin arrangement. We consider two types of the canted spin structures, which can be regarded as intermediate states between the isotropic ferromagnetic ordering (on the one side) and the anisotropic antiferromagnetic ordering of either the layered A-type or the chainlike C-type (on the other side). Our main conclusions are the following: (i) The layered (de Gennes') canting is unstable for small hole concentrations x, and can be destroyed by additional spin rotations within the layers; (ii) However, there are several different regions corresponding to the finite hole concentrations x, inside of which the anisotropic canted spin arrangement can exist; (iii) The transition between the ferromagnetic and the anisotropic canted spin states is characterized by a finite discontinuity of the canting angle. The conditions of the local stability for the A- and C-type antiferromagnetic states with respect to the spin canting in the double-exchange model are also examined. It is shown that they can be expressed in the form of local density of $3z^2-r^2$ states at the Fermi level plus the off-diagonal orbital response. For some examples, results of the model analysis are compared with first-principles band structure calculations performed for the virtual-crystal alloy $\mathrm{La}_{1-x}\mathrm{Ba}_x\mathrm{MnO}_3$ in the local-spin-density approximation. The calculations support the appearance of the canted spin ordering at finite hole concentrations x.

(Submitted to Phys. Rev. B)
Manuscripts available from: igor@jrcat.or.jp

10 Presenting Other Initiatives

NANOPHASE Research Training Network

NANOPHASE (Nanoscale photon absorption and spectroscopy with electrons) is the name of a new Research Training Network, approved for funding (subject to contract) by the European Commission, expected to start on 1 June 2000.

The Network comprises seven teams:

- Fritz Haber Institute, Berlin
- Friedrich Schiller University, Jena
- Lund University
- CNRS/Ecole Polytechnique, Paris
- University of Rome "Tor Vergata"
- University of Valladolid
- University of York

The overall topic of the Network is the theory of nanometre-scale structures - atomic clusters, quantum dots on surfaces or embedded in materials, quantum wires, and molecules adsorbed on surfaces - and the spectroscopic processes that can be used to characterise those structures, their electronic and optical properties, and their growth. Nanostructures are expected to underlie much of future technology, based in most cases on their optical and electronic properties. Our aim is to produce a detailed description and understanding of these properties, together with state-of-the-art ab initio computer simulation software. Research topics will include studies of the spectral function (including quasiparticle energies), optical absorption spectrum and electron energy loss spectrum of various zero- and one-dimensional systems and surfaces on which they are adsorbed. The Network will fund postdoctoral Research Fellowships in each of the seven teams, and a PhD studentship is also available. (See advertisement in the **General Job Announcements** section in this Psi-k newsletter for details.)

Information about Network activities, and the vacant postdoctoral and PhD positions, may be seen at the Network's main web page (`http://www-users.york.ac.uk/~rwg3/nanophase.html`).

Rex Godby (Coordinator) [rwg3@york.ac.uk]

11 SCIENTIFIC HIGHLIGHT OF THE MONTH

Self-Interaction Corrected Electronic Structure of Rare Earths

A. Svane[1], W.M. Temmerman[2], P. Strange[3], Z. Szotek[2] and H. Winter[4]

[1] *Institute of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark.*
[2] *Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U. K.*
[3] *Theoretical Physics Group, School of Chemistry and Physics, Keele University, Keele, Staffordshire, ST5 5BG, U.K.*
[4] *INFP,Forschungszentrum Karlsruhe GmbH, Postfach 3640, D-76021 Karlsruhe, Germany*

Introduction

Solids containing rare earth (lanthanide) and actinide species are characterized by localized atomic-like f^n shells, with large magnetic moments of magnitudes grossly given by atomic Russell-Saunders coupling. The chemical bonding is provided predominantly by the non-f electrons. To describe the electronic structure of such systems from first principles, Skriver et al. introduced the two-fluid model [1] according to which an appropriate number, n, of f-electrons is accomodated in localized core-like f-states, while the remaining valence electrons are described by conventional Local-Spin-Density (LSD) band structure methods, in the subspace of Bloch states composed of s, p and d valence orbitals. In this way the systematics of the lattice structures occurring in lanthanide and actinide metals may be explained.[1] This approach is rather more successful than the straightforward application of LSD, which would describe all valence electrons, including the f's, as Bloch states. The partial occupation of narrow f-bands in this case leads to large cohesive contributions and much too small equilibrium lattice constants. Obviously, the LSD lacks the ability to describe the favourable formation of localized atomic-like f-shells. This is quite natural, since the LSD is derived from the free-electron gas.

The self-interaction corrected (SIC) LSD method constitutes an attempt to repair this deficiency of LSD theory. In the SIC-LSD approximation, the LSD total energy functional is corrected by the subtraction of the self-interaction of each occupied orbital. The occurrence of self-interaction is another deficiency of the LSD energy functional. The exact Kohn-Sham energy functional is self-interaction free.[2] The self-interaction vanishes for Bloch states in the thermodynamic limit, but energetically more favourable states may be found, which benefit from the SIC. Such states are spatially localized on particular atomic positions and the SIC in Eq. (1) becomes equivalent to the energy gained by localization. The question whether localized or delocalized f-states are formed in rare earth systems becomes a question of the size of this localization energy versus the band formation energy. The relative size of these energy contributions may be altered with temperature and pressure. Hence, phase transitions involving changes in f-electron localization may take place as temperature and/or pressure is varied. In previous Newsletters [3] we discussed the successful use of the SIC-LSD to describe localization-delocalization transitions in Ce systems. In this Highlight we will present results obtained for the entire rare earth series for both the metals and the sulphides [6]. Moreover, we shall discuss briefly our results for a large number of Yb compounds [7], including Yb monopnictides, chalcogenides and intermetallics.

The self-interaction of an electron in orbital ψ_α is given by [2]

$$\delta_\alpha = U[n_\alpha] + E_{xc}^{LSD}[n_\alpha], \tag{1}$$

where U and E_{xc}^{LSD} are the Coulomb and exchange-correlation energies of the charge density n_α of orbital ψ_α. Thus the SIC-LSD energy functional is

$$E^{SIC-LSD} = E^{LSD} - \sum_{\alpha}^{occ.} \delta_\alpha. \tag{2}$$

The minimization of this functional within the LMTO method [4] has been described in Ref. [5]. In practice, a fixed number of localized states, n, on all atomic sites is chosen, and the functional minimized with this choice. Consequently, different scenarios (local minima) may be explored corresponding to different assumed valencies. In contrast to the two-fluid model, the present implementation includes those f-degrees of freedom not occupied by localized states in the space available for band states. Therefore, the total occupancy of f-electrons on a given atom will not be an integer, it is the number of *localized* f-electrons which is integral. This leads to a significant reduction of the fluctuation of f-electron number, compared to a full band description, as in LSD. However, the number fluctuation does not completely vanish, as it does in the two-fluid model. The relevance of this 'two kinds of f-electrons' picture was stressed by Gschneidner [8] on the basis of a detailed analysis of experimental data.

In cerium compunds [3] the relevant scenarios are those corresponding to either 1 or 0 localized f-states per Ce atom. The latter coincides with the LSD solution, since when no localized states occur, $E^{SIC-LSD}$ and E^{LSD} are identical. In cerium pnictides and chalcogenides the phase transitions occurring with applied pressure seem to be well described by these two scenarios. Of course other aspects of the physics of cerium compounds (heavy fermion behaviour etc.) is connected with quantum fluctuations between the f^0 and f^1 states, which are still not well described with a single Slater determinant representation as provided by both LSD and SIC-LSD.

Applications

Most of the rare earth atoms are divalent. However, in the metallic state most of the elements become trivalent. In some materials the energy difference between the divalent and the trivalent state is small and by changing some external parameters a transition from one valence state to

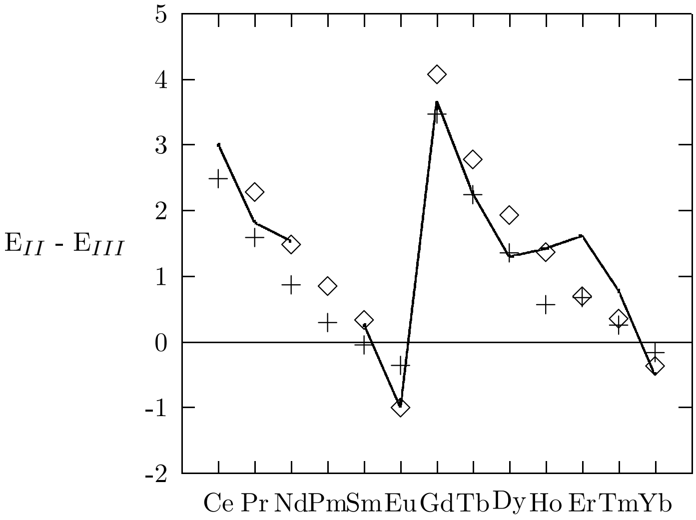

Figure 1: The energy difference (in eV) between the divalent and trivalent state of the rare earth materials. The solid line shows the 'experimental' values for the rare earth metals from Johansson [9]. The diamonds and the crosses are the calculated values for the rare earth metals and the rare earth sulphides, respectively. As the divalent-trivalent energy differences calculated *ab initio* were too negative, they were uniformly shifted by 43 mRy to agree with the observed valence transition pressure of 6 kbar in SmS [10]. This shift also fixes the energy differences for all the other rare earth materials. In particular, for EuS and YbS we find valence transitions occurring at 184 and 75 kbar, respectively, while experimentally, transitions occur at ~ 160 and ~ 100 kbars, respectively.[11]

the other occurs. Perhaps the most famous example of this is observed in SmS which exists in the divalent state as a black semiconductor with the rocksalt crystal structure. Under a pressure of about 6 kbars it undergoes a valence transition to the trivalent state. This involves a 15 % decrease in volume, although there is no change in crystal structure, and a transition to a golden metallic state. But the mechanism underlying this transition and the reason for the differing valence states are not well understood. The SIC-LSD calculations presented here allow us to determine both the valency and the lattice parameter as a function of atomic number. We find, that the delocalized band-like f-electrons are found only in the trivalent systems, and if their number exceeds a certain threshold it becomes energetically favourable for these electrons to localize, causing a transition to a divalent ground state.

In the lanthanide series we have considered configurations f^n and f^{n+1} of the lanthanide atom with n chosen so as to represent trivalent and divalent rare earth atoms, respectively.[6] Here we define valency as the number of electrons per atom available for band formation. In Fig. 1 we show the energy difference between these two valency configurations as a function of the lanthanide elements. The figure shows results for both the pure metals and for rare earth sulphides, and the numbers are compared to the experimental estimates. [9] For both the elemental metals and the sulphides the trends are the same, and also the same for the first and second half of the series. In the beginning the trivalent state is very much favoured over the divalent state, but the latter becomes progressively more favourable as we proceed through the

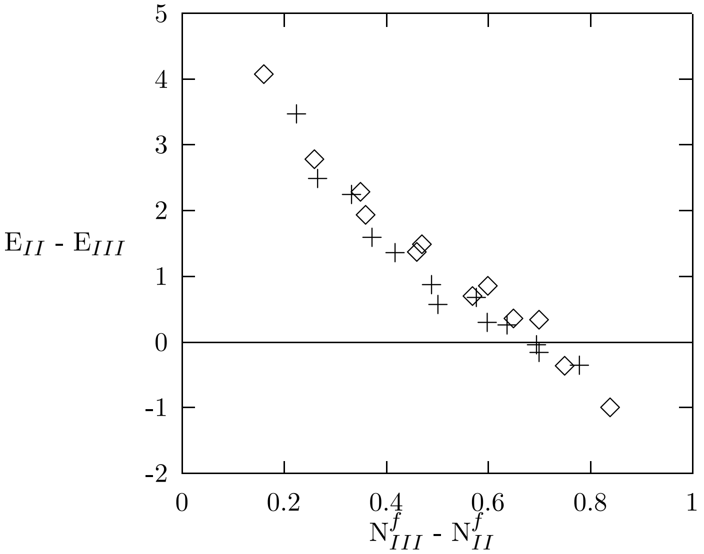

Figure 2: The energy difference (in eV) between the divalent and trivalent state of the rare earths and their sulphides plotted as a function of the difference in the number of band-like *f*-electrons. Each point in this figure represents one rare-earth element (diamonds) or one rare earth sulphide (crosses). The fact that the metals and the sulphides fall on the same line strongly suggests that it is the number of delocalized *f*-electrons that determines the valence. When the difference becomes ∼ 0.7 or more, the divalent state is more stable.

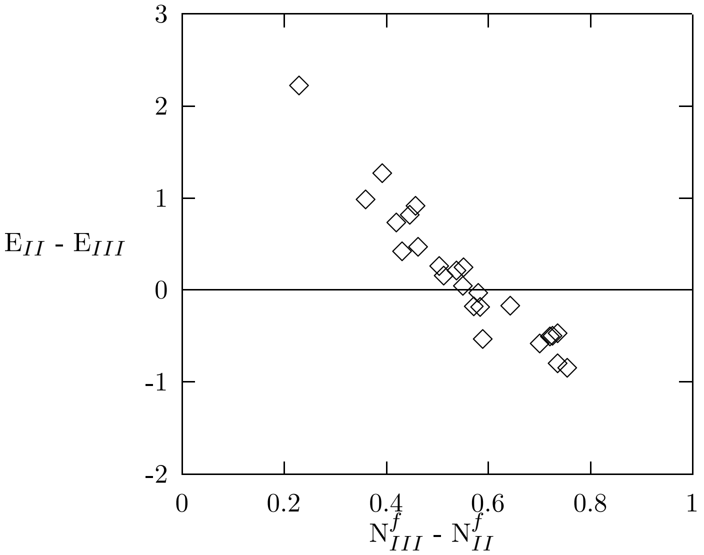

Figure 3: The energy difference (in eV) between the divalent and trivalent configurations of Yb compounds versus the total *f* occupancy difference between the trivalent and divalent configurations, as given by the SIC-LSD approach. The data points correspond to YbCd, YbZn, YbPd, YbRh, YbRu, YbIr, YbAg, YbAu, $YbAl_3$, $YbPd_3$, Yb_3Pd, YbIn, YbTe, YbSe, YbS, Yb, YbSb, YbBi, YbBiPt, YbN, YbP, YbAs, YbO, $YbAl_2$.

series. Around Sm the two valencies are nearly degenerate, and for Eu and EuS the divalent state has lowest energy. In the second half of the series, when the minority spins of the f-shell are being filled the same things happen: for Gd the trivalent configuration is strongly favoured but towards the end the two valencies are again nearly degenerate, with the divalent state favoured in Yb and YbS. The results are seen to reproduce the experimental estimates quite well. These trends are caused by the position of the f-resonance for the majority (minority) spin band in the first (second) half of the lanthanide series. When the atomic number Z of the rare earth atom is increased, the f-resonance moves down a bit with respect to the $6s$-$5d$ conduction states. Consequently, progressively larger f-hybridization into the conduction bands occurs. In Fig. 2 we correlate the number of f-electrons in the conduction bands in the trivalent configuration with the divalent-trivalent energy difference. A neat linear relationship is observed. When ~ 0.7 or more f-electrons are accomodated in the conduction states, it becomes energetically more favourable to occupy one additional f-electron in a localized state, i. e. to switch to the divalent configuration.

Yb compounds, similarly to Ce compounds, exhibit valence fluctuations, in this case between trivalent (f^{13}) and divalent (f^{14}) configurations. We have investigated a large number (24 systems) of Yb compounds [7] and again find that the valence stability depends on the degree of hybridization of the last f-electron into the conduction band in the trivalent Yb compounds. This is illustrated in Fig. 3. When the number of band f electrons in the trivalent configuration exceeds a value ~ 0.7, the divalent Yb configuration is favoured.

The Yb compounds considered here can be divided into three groups, according to the energy difference between the divalent and trivalent Yb configurations. The group of strongly trivalent compounds comprises YbN, YbP, YbAs, YbRu, YbRh, YbIr, $YbAl_3$ and $YbPd_3$. For this group the trivalent configuration is favourable over the divalent configuration by more than 20 mRy per Yb atom. In addition, the calculated equilibrium volumes for the trivalent configuration agree well with experimental volumes (within an average 3.4 % deviation). In comparison, the calculated equilibrium volumes for the divalent Yb configurations are an average 14 % too large. The second group consists of the strongly divalent Yb compounds, encompassing YbO, Yb, YbS, YbSe, YbTe, Yb_3Pd and YbIn. Here the divalent Yb configuration is favoured over the trivalent by more than 20 mRy. The calculated volumes for the divalent configuration agree within an average 2 % deviation with the experimental volumes, whereas the equilibrium volumes for the trivalent state are lower by 12 % on the average.

The remaining compounds are characterized by having the energy of the divalent and trivalent configurations equal within 20 mRy. Hence effects of valency fluctuations may start to be important. We have found, however, that the weakly divalent compounds, the intermetallics YbCd, YbZn, YbAg and YbAu, are in fact well described by the divalent configuration, as evidenced by the agreement between the calculated and experimental volumes (general agreement within 3 %). Hence, for these compounds there seems to be no need for additional cohesive contribution stemming from valence fluctuations. Interesting behaviour is to be expected when pressure is applied to these materials, since the trivalent state will then become more favourable. We are, however, not aware of any pressure experiments done on any of these Yb intermetallics. Finally, the compounds YbPd, YbSb, YbBi, YbBiPt and $YbAl_2$ are weakly trivalent, i.e. according to the calculations the trivalent state is favoured by less than 20 mRy. Among these, YbBiPt and

$YbAl_2$ are known heavy-fermion compounds, and YbPd is believed to be mixed valent system, with approximately equal proportions of Yb^{2+} and Yb^{3+} ions. Hence, for compounds in this group the valence fluctuation phenomena are most significant.

We conclude that the SIC-LSD does provide a reliable scheme for calculating the valence stability in Yb compounds, maybe with an error of the order of 10-20 mRy. Given the complexity of the phenomena studied, such an error is quite reasonable and acceptable.

Conclusions

The SIC-LSD method represents a rather simple implementation of the two-fluid model of Skriver et al., however, with an important extension of allowing for f-hybridization into the conduction bands. As a consequence two kinds of f- electrons are present in rare earth systems, as argued earlier by Gschneidner [8]. The method describes successfully the equilibrium lattice constants of rare earth metals and sulphides, where the LSD generally leads to much too small lattice parameters. However, several questions remain, since the method can only treat ideal f^n shells with n integral. Valence fluctuations and the gradual delocalization of the f manifold is therefore still outside the scope of the method, and if significant energy contributions are associated with such effects, this will have to be considered separately. In addition, one may question whether the self-interaction correction (1) represents the appropriate localization energy. It obviously has the correct order of magnitude, otherwise the valence transitions in cerium compounds and the trends of Fig. 1 would not come out correctly. On the other hand, the calibration needed in Fig. 1, or the $\sim$ 10 mRy overestimation of the stability of the Yb^{3+} configurations over Yb^{2+} configurations, may be due to an error in the appropriate localization energy. Also, other aspects of the atomic coupling energies, like the orbital polarization energy [12], may be important to consider.

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