

# $\Psi_k$ Newsletter

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

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# 1 Editorial

In this *Newsletter* we would like to turn your attention to the information on the Psi-k 2000 Conference which can be found in the **General News** section. There we give also some travel information on how to get to Schwäbisch Gmünd. In subsequent sections readers can find a number of reports on workshops and collaborative visits, job and workshop/conference announcements, and abstracts of newly submitted papers. Please note that in this *Newsletter* we publish the **Mid-term Report on the ESF Psi-k (STRUC) Programme**. The scientific highlight is by Igor Abarenkov (*St. Petersburg*) and Volker Heine (*Cambridge*) on "**A new theorem for embedding with application to a new hybrid method for difficult composite systems marrying configurational interaction and density functional calculations**". Please see the table of contents for further details.

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

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

The above contains 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.

	<b>function</b>
<a href="mailto:psik-coord@daresbury.ac.uk">psik-coord@daresbury.ac.uk</a>	messages to the coordinators, editor & newsletter
<a href="mailto:psik-management@daresbury.ac.uk">psik-management@daresbury.ac.uk</a>	messages to the NMB of all Networks
<a href="mailto:psik-network@daresbury.ac.uk">psik-network@daresbury.ac.uk</a>	messages to the whole $\Psi_k$ community

Dzidka Szotek and Walter Temmerman  
e-mail: [psik-coord@dl.ac.uk](mailto:psik-coord@dl.ac.uk)

## 2 General News

### 2.1 Psi-k 2000 Conference

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

Schwäbisch Gmünd, 22-26 August, 2000

Today, May 31, is the deadline for early registrations. After this date the conference fee will be increased from 160 to 250 EURO. As for today we have over 380 registrations to the conference.

#### Conference duration

Please note that the conference will commence with registrations on Tuesday afternoon (August 22), while talks will start on Wednesday morning (August 23). The conference will finish on Saturday (August 26) at about 18:00.

#### Registration and conference fee

Note also please that before it is known how many have registered and offered a contribution, it will be impossible to decide how many can receive any financial support. So, if you have an intention to come to the conference, please do register as soon as possible. Please note that, unless you are a plenary or invited speaker, **paying the conference fee is a very important part of the registration process!** It is important that also the plenary and invited speakers register and submit abstracts.

#### Contributed Papers

Please do try to submit your abstracts while registering to the conference. Note also please that only after finalizing registrations and collecting all abstracts we shall be able to inform all on whether their contributions have been accepted as a short talk or a poster. We plan to be able to provide you all the relevant details on symposium and type of presentation of your contribution in the second half of June.

## **Financial Support**

Judging by the amount of requests for funding we shall only be able to provide partial financial support. Those who receive support will be informed by e-mail in the second half of June.

## **How to get to Schwäbisch Gmünd**

From the Stuttgart Airport: Follow the signs for the S-Bahn (a large S sign). The train station in the Airport is situated in the underground of the arrival building. There you need to buy a ticket to Schwäbisch Gmünd from the automatic ticket machine. The single ticket costs 20.20 DM. It is possible to use bank notes and the machine gives change in coins. There are two trains (S2, S3) that one can take. At the Bad Cannstatt stop, the first one after the Hauptbahnhof, the main railway station, leave the train and change to the train for Schwäbisch Gmünd (direction Aalen). The whole journey time from the airport to Schwäbisch Gmünd is just over an hour.

To travel from the Stuttgart Airport to the main railway station (Hauptbahnhof), one needs to take S-Bahn (trains S2 or S3). The price of the ticket is 4.80 DM. The journey takes 27 minutes. The frequency of trains is at least three per hour from 5:00 until 24:00. You will arrive at the underground level of the 'Hauptbahnhof'.

If you are starting your journey from the Stuttgart main railway station or you want to break your journey to visit the town and then follow to Schwäbisch Gmünd, you can buy tickets for the train to Schwäbisch Gmünd at the street level, on the right hand side of the train station (facing the station building in the street outside). Tickets are also available on the train. The price is 15.40 DM (return ticket 30.80 DM) for a second class ticket. The platforms for Schwäbisch Gmünd are one level above the street level. The track (=Gleis, in German) number from which the train leaves can be found on the timetables in the station. There are two timetable posters: Abfahrt (= departure) and Ankunft (= arrival). There is at least one train per hour from 5:51 until 23:22. The journey takes about 40mins.

Please that detailed information on the train connections to Schwäbisch Gmünd can be found on the web page of the Deutsche Bahn. Note that the Psi-k web site provides a link to the Deutsche Bahn web site.

A taxi from the Stuttgart Airport to Schwäbisch Gmünd costs about 130 DM, although one could try to negotiate a fixed price which might then be somewhat lower.

## **Web Site**

Details of the programme (provisional speakers, etc.) are given below and can also be

found on our Web site:

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

The final programme and the book of abstracts will be distributed at the end of July, possibly together with the next Psi-k newsletter.

The above site also contains information about contributing papers, registration and accommodation. Please do remember to book your accommodation by printing off and filling in the booking form available on the above web page.

### **Plenary talks, symposia and invited speakers**

#### **Plenary talks**

Hardy Gross	New Directions in DFT
Norton Lang	DFT Studies in Molecular Electronics
Peter Levy	Magnetotransport in Multilayered Structures
Matthias Scheffler	The cutting edge: surfaces and their role in materials' properties

#### **Invited talks**

#### **Symposium on "Bandstructure Methods"**

O.K. Andersen	NMTOs
P. Dederichs	Conceptual improvements of the KKR method
E. Krasovskii	Electronic structure of bulk and semi-infinite crystals by the extended LAPW-kp method
N. Marzari	Localized Wannier functions in extended systems: theory and applications
T. Saha	Tight-Binding modelling and generation of first-principles Wannier-like orbitals using the new NMTO scheme
H. Skriver	Exact MT orbitals in the spherical cell approximation

#### **Symposium on "Correlated systems"**

S. Ezhov	Orbital occupation, local spin and exchange interactions in V <sub>2</sub> O <sub>3</sub>
A. Georges	Introduction to Dynamical Mean Field Theory and its possible use in realistic calculations
O. Gunnarsson	Resistivity of alkali-doped fullerenes: Lack of saturation at high temperatures
A. Liechtenstein	Beyond LDA
A. Mookerjee	Response functions and the recursion method

- W.E. Pickett Coexistence of High-Temperature Superconductivity and Magnetism:  
RuSr<sub>2</sub>GdCu<sub>2</sub>O<sub>8</sub>
- I. Solovyev Aspects of charge, spin and orbital ordering in manganites

### **Symposium on "DFT"**

- R. Resta Macroscopic polarisation and electron localisation in extended systems
- J. Snijders TDDFT results for solids
- L. Vitos Kinetic and exchange functionals in the local Airy gas approximation

### **Symposium on "Excited States/Quasiparticles"**

- S. Louie Ab initio optical absorption and quasi particle spectra
- L. Reining Application of Greens function methods to calculation of excited states
- A. Rubio Lifetimes of hot electrons in metals
- R. Del Sole Ab initio calculation of optical properties of surfaces
- W. Wolf Screened exchange FLAPW calculations of optical properties

### **Symposium on "f-Electron Systems"**

- M.S.S. Brooks Relativistic effects in f-electron systems
- L. Nordström Magnetism of the rare earth from first principles calculations
- A. Svane Self-Interaction Corrected Electronic Structure of  
Lanthanides and Actinides

### **Symposium on "Interfaces"**

- S. Koestlmeier Ab-initio Investigation of Metal/Ceramic Bonding:  
Metal/Spinel Interfaces
- A. Pasquarello Silicon and its Oxide
- W. Sigle(\*) To be announced

II

### **Symposium on "Large Systems/O(N)"**

- D. Bowler CONQUEST: codes and applications
- S. Goedecker Linear scaling methods for electronic structure
- P. Ordejon Applications of SIESTA
- D. Pettifor Bond-order potentials: bridging the electronic to  
atomistic modelling hierarchies

### **Symposium on "Magnetism"**

- I. Abrikosov Understanding the INVAR effect in Fe-Ni alloys

- S. Baroni Magnons in real materials from a generalized adiabatic decoupling scheme
- S. Blügel Magnetic phenomena at surfaces
- M. Pederson Molecular magnets: Anisotropy Energies and Resonant Tunnelling Fields within DFT
- J. Staunton Dynamical spin susceptibility of alloys
- L. Udvardi Structure of Bloch walls: Heisenberg model vs. RSP calculations

### **Symposium on "Magnetoelectronics"**

- A. Barthelemy Magnetic tunnel junctions: experimental results and open questions
- W.H. Butler Spin-dependent tunneling in epitaxial Fe(100)—MgO—Fe(100)
- J. Kudrnovsky Ab initio theory of transport
- I. Mazin Is spin polarization a measurable quantity?
- I. Mertig Theory of GMR
- N. Papanikolaou Spin-dependent tunneling in metal-insulator junctions
- E. Tsybal Spin polarisation of conductance in magnetic tunnel junctions

### **Symposium on "Materials Science"**

- G. Bihlmayer The FLAPW method applied to complex magnetic systems
- N.E. Christensen New High-Pressure Phases in Alkali Metals and group IV Semiconductors
- L. Colombo To be announced
- Z. Fang Applications of ultrasoft pseudopotentials to 3d and 4d transition metal oxides
- K. Fichtorn Island nucleation in thin film epitaxy - a multiscale study
- M. Gillan How to find the chemical composition of the Earth's core using DFT
- O. Jepsen High pressure phases
- G. Kresse Fast all-electron ab-initio molecular dynamics
- R. Martonak Ab-initio molecular dynamics with a pressure reservoir: simulation of pressure-induced transformations in silicon clusters

### **Symposium on "Molecular and Biological Systems"**

- E. Artacho Large scale calculations on DNA and proteins
- P. Carloni Drug-target interactions in anti-AIDS therapy: an ab initio approach
- B. Lesyng Mesoscopic Poisson-Boltzmann and Quantum-Classical Studies of Enzymatic Reactions
- C. Rovira Active centre in oxygen-carrying proteins

U. Roethlisberger First-Principles Modeling of Enzymes  
M. Segall Biological applications of the CP method

### **Symposium on "Nanostructures and Quantum-dots"**

M. Nardelli Theory of electronic and transport properties of carbon nanotubes  
D. Portal-Sanchez Monoatomic gold wires  
T. Todorov Current-induced mechanical effects in atomic-scale conductors  
A. Williamson Calculations of multiple excitons in InAs quantum dots

### **Symposium on "Optimized Effective Potential"**

E. Engel Description of dispersion forces with implicit density functionals  
A. Goerling Advances in DFT by treating exchange exactly  
M. Seidl Strong-interaction limit of DFT: its simplicity and its relevance for electron systems

### **Symposium on "Polymers and Optoelectronics"**

W. Barford Conjugated Polymers  
M. Cote New polymers for optoelectronic applications  
B. Delley Structural switching in molecular complexes  
I. Frank Chemical reaction induced by mechanical stress: ab-initio simulations  
E. Molinari Excitons in polymer chains and crystals: an ab initio approach  
H. Weiss DFT as a versatile tool in industrial catalysis research

### **Symposium on "Quantum Monte Carlo"**

M. Caffarel New Developments in Quantum Monte Carlo calculations of observables  
C. Filippi Constructing optimal orbitals for QMC  
R. Needs Accurate QMC calculations for ground and excited states  
S. Sorella Strongly correlated electrons and QMC

### **Symposium on "Semiconductors"**

P. Bloechl On the calculations of defects in silica  
M. Hierlemann To be announced  
P. Kratzer From DFT studies to growth simulations: Modeling molecular beam epitaxy of arsenide compound semiconductors  
J. Ortega Electron correlation effects and dynamical fluctuations at semiconductor surfaces: Sn/Si(111) and Sn/Ge(111)  
M. Pesola Oxygen-related Defects in Si and GaAs

- K. Schroeder      Theory of surfactant-mediated growth  
 C. Van de Walle    Properties of GaN surfaces: the role of H

### **Symposium on "Superconductivity"**

- J.F. Annett    Exotic superconductors  
 K. Capelle    Relativistic effects and dichroism in superconductors  
 E. Pavarini    Hyperfine fields in cuprate superconductors  
 D. Singh      Is singlet and triplet superconductivity incompatible?  
 Z. Szotek      Quasiparticles in d-wave superconductors

### **Symposium on "Surfaces"**

- A. Alavi        Chemistry at metal surfaces from density-functional theory:  
                   successes, failures and challenges  
 A. Bogicevic    Atom dynamics and diffusion on surfaces  
 V. Fiorentini    To be announced  
 J. Kollar        Stability of metal surfaces: Surface, step and kink formation energies  
 Y. Morikawa    Ab initio study of methanol synthesis over Zn-deposited Cu surfaces  
 J. Nørskov      Catalysis from first principles  
 C. Stampfl      Ab initio modelling of T-programmed desorption of molecules  
                   from metallic surfaces  
 H. Toalhout    Periodic trends and synergy effects in hydrodesulfurization catalysts:  
                   recent findings based on electronic structure calculations

### **Symposium on "Spectroscopies"**

- M. Alouani      Calculated Magnetic X-ray circular dichroism of binary alloys  
 S. Crampin      Calculations of second harmonic generation from magnetic interfaces  
 K. Karlsson    Cuprate core-level line shapes for different Cu-O networks  
 N. Lorente      First principles calculations of single molecule vibrational  
                   spectroscopy and microscopy  
 A. Paxton        Near edge structure in energy-loss spectroscopy of transition metal nitrides:  
                   some many electron and magnetic effects using density functional theory  
 J. Redinger      First-Principles Simulation of Scanning Tunneling Microscopy and Spectroscopy  
 G. van der Laan    Configuration interaction and correlation in magnetic 3d metals

(\*) To be confirmed

## 3 News from the TMR1 Network

### ”Interface Magnetism”

#### 3.1 Reports on Workshops

##### 3.1.1 Report on Prague GMR/TMR miniworkshop

The Prague GMR/TMR miniworkshop took place on April 13-14, 2000 at the Institute of Physics of the Academy of Sciences of the Czech Republic. The co-organizers of the miniworkshop were the Technological foundation of the Czech Republic and the TMR1 Network 'Interface magnetism'. It was attended by the following persons: C. Blaas (Vienna); V. Drchal, J. Kudrnovský, and F. Máca (all from Prague); I. Turek (Brno); P.H. Dederichs, M. Freyss, and N. Papanikolaou (all from Jülich); J. Binder, I. Mertig, I. Riedel, and P. Zahn (all from Dresden); and J. Henk and A. Ernst (from Halle).

The aim of the miniworkshop was to discuss the current status of the giant and tunneling magnetoresistances (GMR and TMR), in particular, its *ab initio* formulations. The emphasis was also put on purely technical aspects of calculations which usually remain 'hidden' in publications and/or in conference talks. In some cases, also unfinished and open results were presented. In total 13 talks were divided into three subjects, namely to the TMR, GMR, and electronic-structure sections (each lasting one half-day) with intensive discussions.

All participants were from cities close to Prague which has allowed to reduce significantly travel expenses (Jülich group was in Prague for one week in the framework of the Czech-German collaborative grant). All participants are partners of the future RT-Network on 'Computational Magnetoelectronics'.

#### **The program of the miniworkshop:**

##### **The TMR-section**

N. Papanikolaou et al.:

*Complex Band Structure and Tunneling through Metal/Insulator/Metal Junctions*

J. Henk and P. Bruno:

*A layer-KKR approach to Bloch-wave transmission applied to spin-dependent tunneling*

F. Máca and W.A. Hofer:

*Comparison between ab-initio simulations and STM-images*

V. Drchal and J. Kudrnovský:

*Tunneling magnetoresistance and interface states*

I. Riedel et al.:

*Transmission coefficients - a new formalism*

### **The GMR-section**

J. Binder et al.:

*Ab initio calculations of Giant MagnetoResistance*

J. Kudrnovský et al.:

*Ab-initio theory of perpendicular transport in complex layered systems*

C. Blaas et al.:

*Theoretical evaluation of magneto transport properties in Co/Cu/Co*

F. Erler et al.:

*Giant MagnetoResistance of finite multilayers*

### **The electronic structure-section**

M. Freyss et al.:

*Electronic and magnetic properties of Fe/semiconductor tunnel junction*

I. Turek et al.:

*Electronic Structure and Transport Properties of Fe/Si/Fe(001) Trilayers*

P. Zahn and I. Mertig:

*Ab initio description of TMR electrodes Fe, Co, and Ni*

A. Ernst et al.:

*GW Approximation for Study of Electronic Structure of Oxides*

J. Kudrnovský and P.H. Dederichs

## 3.2 Reports on Visits to Conferences/Workshops

### Report on A Conference Participation:

**”18th general conference of the Condensed Matter  
Division of the European Physical Society”  
Montreux, CH, March 13-17, 2000**

The 18th CMD conference was attended by more than 1100 people, mostly from Europe and Japan. The conference was very exciting and gave an overview of the current research activities in condensed matter physics. In short, the interest for new materials and the theoretical explanation of their properties is rapidly increasing.

The plenary sessions concentrated on the improvements over the last years of important new domains in physics, like the quantum computing presented by J.S. Tsai (NEC, Tsukuba), the use of nanotubes as quantum wires by C. Dekker (Delft), the quantum mirages by H.C. Manoharan (IBM, Almaden) and the connection between X-rays and magnetism presented by C. Vettier (ILL, Grenoble). Focused sessions and mini-colloquiums gave to the present scientists the occasion to focus on more specific subjects like the recent advances in computational physics, where E.K.U Gross (Würzburg) presented a new density functional theory for semiconductors, and the advances in the field of spin-dependent transport in magnetic nano-systems, where J.M. de Teresa presented the work carried out in CNRS/Thompson-CSF on manganites. In the mini-colloquium on low dimensional magnetic systems, W. Wulphenkel (Halle) presented the recent developments in the spin-polarized scanning tunneling microscopy and G. Tatara (Osaka) in the connection between resistivity and domain walls for nano-magnets. Many other contributions would deserve to be noticed.

Iosif Galanakis (TMR-PhD student) presented his work on the effect of the local environment on the magnetic properties of a material showing uniaxial anisotropy. On the other hand Alberto Debernardi (TMR Post-Doc) presented some preliminary results of his work on the lattice properties of bulk metals. For the two participants from Strasbourg, it has been an unique opportunity to have a wide and deep view on the latest developments in condensed matter physics in Europe.

Iosif Galanakis

Alberto Debernardi

## 4 News from the TMR2 Network

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

#### 4.1 Reports on Workshops

##### 4.1.1 Report on BdG Workshop

#### The VI Bristol Workshop on the Bogoliubov-de Gennes Equations

Burwalls, Bristol, United Kingdom

April 14-16, 2000

*Sponsors: The European Science Foundation (ESF), TMR2 (EU) Network, and the Computational Collaborative Project 9 (CCP9) (UK)*

The aim of the workshop was to bring together various communities whose work involved the Bogoliubov-de Gennes (or related) equations. Working in different fields such as superconductivity, superfluidity and nuclear physics, these groups do not cross paths in their daily research and have found this forum to exchange ideas very inspiring.

The workshop took place on the weekend of April 14-16 at Burwalls, a conference centre of Bristol University. Due to the generous support by the European Science Foundation and the Training and Mobility of Researchers (TMR) network on "Electronic Structure of Complex Systems", which has a superconductivity node at Würzburg, on this occasion we were able to invite American and outside-EU European speakers, as well as, the customary UK and EU participants. As a consequence, it was more than usually lively meeting. Although the emphasis remained on superconductivity, the talks of Wilkin on rotating superfluids, and that of Bertech on nuclei with high angular moments gave us fresh insights on pairing. The discussions on superconductivity were focused on the effects of large magnetic fields, finite size effects (mesoscopics), exotic pairing, cross-over to Bose-Einstein condensation, disorder and high temperature superconductivity. For further information below we record the full program and a list of participants.

#### Programme

## **April 14, Friday**

7:30 pm Welcome and Buffet Dinner

## **April 15, Saturday**

### 9:00-10:00 am **Density Functional Theory for Superconductors**

Gross, E.K.U. (Würzburg + Bristol): Density Functional Theory for Superconductors: Calculating  $T_c$  from First Principles.

Capelle, K (Sao Carlos): BdG Equations for Spin-Density-Wave States.

### 10:00-11:00 am **Bose-Einstein Condensation**

Wilkin, N K (Birmingham): Condensation of 'Composite Bosons' in Rotating BEC

Micnas, R (Poznan): BCS-LP Crossover and Phase Fluctuations in Short Coherence Length Superconductors

11:00-11:30 am Coffee

### 11:30-1:00 pm **Exotic (non s-wave) Pairing**

Annett, J F (Bristol): Frustrations in d-wave Superconducting Circuits: -ring Behaviour

Szotek, Z (Daresbury): Quasi-Particles in d-wave Superconductors

Bertsch, G (Seattle): Finite System Pairing from a Nuclear Physics Perspective

1:00-2:00 pm Lunch

### 2:00-4:00 pm **Mesoscopic Superconductivity**

Lambert, C, Taddei, F, McCan, E and Newman, C (Lancaster): Phase-Coherent Transport in Nanostructures

Büttiker, M (Geneva): Injectives, Distribution Functions and Current-Current Correlations in NS Junctions

Martin, A (Geneva): Time Dependent Bogoliubov-de-Gennes Equations and NS interfaces

Zaikin, A (Karlsruhe): Superconductivity in One Dimension: New Quantum Phase Transition

4:00-4:30 pm Coffee

### 4:30-6:30 pm **Quasi-particles in Vortices and Interfaces**

Kümmel, R (Würzburg): Andreev Scattering, Vortex Motion and Josephson Effects

Duncan, K (Bristol): Semiclassics for Superconductors

Hedegard, P (Copenhaguen): SO(5) Theory and Insulating Vertex Cores

6:30-7:30 pm Dinner

7:30-8:00 pm Tesanovic, Z: Quantum Dynamics of Vortices and Quasiparticles in the Superconducting State

**April 16, Sunday**

9:00-10:00 am **Mechanisms of Pairing**

Jarrell, M (Cincinnati): d-wave Superconductivity in the Hubbard Model

Monthoux, P (Cambridge): P-wave and D-wave Superconductivity in Quasi-2D and 3D Metals

10:00-11:00 am **Preformed Pairs**

Quintanilla, J (Bristol): Are there d-wave composite bosons?

Wallington, J P (Leuven): BSC-Bose Einstein Crossover in a Lattice Model of d-wave SL

Alexandrov, A S (Loughborough): Gap, Subgap Tunneling and Vortex Structure in the Cuprates

11:00-11:30 am Coffee

11:30-12:30 pm **Disordered Superconductors**

Györfy, B L (Bristol): Superconductors in  $d=\infty$

Litak, G (Lublin): P-wave Pairing in Disordered Ruthenates

1:00-2:00 pm Lunch

End of Workshop

**List of Participants**

A.S. Alexandrov (Loughborough)	B. Andersen (Copenhagen)
J.F. Annett (Bristol)	S. Bailey (Lancaster)
J. Bertech (Seattle)	M. Buttiker (Geneva)
K. Capelle (Würzburg+Sao Carlos)	C. Dent (Loughborough)
P. Dolby (Lancaster)	K. Duncan (Bristol)
L. Fast (Würzburg)	H. Fehrman (Lancaster)
E.K.U. Gross (Bristol+Würzburg)	J.M.F. Gunn (Birmingham)
B.L. Gyorffy (Bristol)	P. Hedegard (Copenhagen)
M. Jarrell (Cincinnati)	R. Kümmel (Würzburg)
C. Lambert (Lancaster)	G. Litak (Lublin)
M. Lüders ((Daresbury)	M. Marques (Bristol)
A. Martin (Geneva)	S. Massidda (Cagliari)
E. McCann (Lancaster)	R. Micnas (Poznan)
P. Monthoux (Cambridge)	R. Moradian (Bristol)
C. Newman (Lancaster)	N. Petterson (Lancaster)
B. Powel (Bristol)	J. Quintanilla (Bristol)
R. Scovell (Bristol)	P. Shakespeare (Bristol)
Z. Szotek (Daresbury)	F. Taddei (Lancaster)
W.M. Temmerman (Daresbury)	Z. Tešanovic (Baltimore)
A. Vetter (Würzburg)	J. Wallington (Bristol+Leuven)
N. Wilkin (Birmingham)	H. Winter ((Daresbury+Karlsruhe)
K. Wysokinski (Lublin)	A. Zaikin (Karlsruhe)

(Balazs L. Gyorffy)

#### 4.1.2 Report on Mini-Workshop at Daresbury

## Electronic Structure and Magnetism in Strongly Correlated Electron Systems

Daresbury Laboratory, May 23, 2000

This one-day miniworkshop brought together people involved in *ab-initio* calculations of the electronic structure of strongly correlated systems, based on the self-interaction corrected local-spin-density approximation. Seminars were given on the ongoing research projects in the various groups. A broad range of applications was represented, including *4f* and *5f* elements and compounds, and *3d* transition metal oxides, with contributions on both surfaces of NiO, manganites and high  $T_c$  superconductors. The informal talks were interspersed with lively discussions and fruitful exchanges of ideas.

### Programme

- 11:00 - 11:30 Axel Svane (Aarhus)  
*Electronic and Magnetic Properties of Yb Compounds and Actinides*
- 11:30 - 12:00 Leon Petit (Aarhus)  
*Electronic and Magnetic Properties of Am-Pnictides*
- 12:00 - 12:30 Paul Strange (Keele)  
*Electronic and Magnetic Properties of Eu-Chalcogenides*
- 12:30 - 13:30 Lunch
- 13:30 - 14:00 Diemo Ködderitzsch (Halle)  
*Electronic and Magnetic Properties of NiO Surfaces*
- 14:00 - 14:30 Rik Tyler (Sheffield)  
*Electronic and Magnetic Properties of Manganites*
- 14:30 - 15:00 Walter Temmerman (Daresbury)  
*Electronic and Magnetic Properties of YBCO*

### List of participants

- E. Arola (Keele)  
G. van der Laan (Daresbury)  
D. Ködderitzsch (Halle)  
M. Lüders (Daresbury)  
L. Petit (Aarhus)

P. Strange (Keele)  
A. Svane (Aarhus)  
Z. Szotek (Daresbury)  
W.M. Temmerman (Daresbury)  
R. Tyer (Sheffield)  
H. Winter (Karlsruhe/Daresbury)

(Axel Svane)

### 4.1.3 Report on FPLAPW Workshop

## Sixth W I E N - W O R K S H O P

# Full-Potential LAPW Calculations with the WIEN97 Code

*Vienna University of Technology, Vienna, Austria*

April, 26-29, 2000

*Chairman:* K. Schwarz (TU Wien)

### **Sponsors:**

TMR(2) Psi-k Network and ESF (European Science Foundation) Programme  
TU Wien and its Computing Center

This sixth workshop was 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. The workshop had two parts: an introduction to the WIEN97 program package with hands-on exercises for novice users (2 days), and the presentation and discussion of various scientific results obtained with the FP-LAPW or related methods (2 days). It was attended by 64 researchers from nineteen countries.

The scientific programme of part I covered a short introduction (by K. Schwarz) to Density Functional Theory (DFT), band structure methods in general and the LAPW method, with corresponding algorithms and features, in particular. The outline and the handling of the program package was described in detail by P. Blaha assisted by J. Luitz and C. Ambrosch-Draxl, who illustrated the graphical user interface by performing the corresponding calculations for a simple test case. In addition to this demonstration the participants had plenty of time to run WIEN97 on several workstations in four exercise sessions. This arrangement was well accepted by the novice WIEN97 users.

In the second part applications directly or indirectly related to the WIEN97 package were presented as lectures or posters illustrating many interesting results such as phase transitions and relative phase stability, LDA+U for strongly correlated systems, spin-orbit splitting, electric field gradients, Fermi surfaces, photoemission spectra and chemistry at surfaces. In addition to these topics computational aspects were discussed, e.g. fine grain parallelization of the code (a coarse grain version on the k-point level is already available).

We have received very positive reactions from the participants who told us that they found the workshop very stimulating and scientifically enriching. They liked the balance of this workshop in terms of introduction, lectures, program handling, exercises and presentation of results. From all the informal discussions which took place it can be expected that several interesting European collaborations will evolve from this workshop.

### List of Participants

Jürgen Almanstötter (OSRAM, Schwabmünchen, Germany)  
Claudia Ambrosch (University Graz, Austria)  
Christian Ammon (University Erlangen, Germany)  
Bouhafs Bachir (University of Sidi Bel Abbes, Algeria)  
Felix Baumberger (Universitaet Zuerich, Schweiz)  
Petra Becker (University of Cologne, Köln, Germany)  
Uwe Birkenheuer (MPI Dresden, Germany)  
Peter Blaha (TU Wien, Austria)  
Bachir Bouhafs (University of Sidi Bel Abbes, Algeria)  
Marc Bovet (Université de Fribourg, Switzerland)  
Guillermo Bozzolo (Ohio Aerospace Institute, Brookpark, USA)  
Igor Burlakov (TU Freiberg, Germany)  
Miroslav Cerny (Brno University of Technology, Czech Republic)  
Qing Chen (Royal Institute of Technology, Stockholm, Sweden)  
Shuiquan Deng (Max-Planck-Institute FKF, Stuttgart, Germany)  
Alejandro Diaz-Ortiz (University of Texas at Austin, Austin, USA)  
Martin Divis (Charles University, Prague, Czech Republic)  
Bernd Eberhard (Universität Augsburg, Germany)  
Jussi Enkovaara (Helsinki University of Technology, Finland)  
Claudia Felser (J.G.Universität Mainz, Germany)  
Anders Froseth (Physics NTNO, Trondheim, Norway)  
Grzegorz Gajewski (University of Wroclaw, Poland)  
Shiwu Gao (Chalmers University of Technology, Gothenburg, Sweden)  
Jorge Garces (Centro Atomico- Bariloche, Rio Negro, Argentina)  
Gabriela Grad (TU Wien, Austria)  
Ccile Hébert (TU Wien, Austria)  
Henning Henke (Universität Karlsruhe, Germany)  
Moritz Hoesch (Universität Zürich-Irchel, Switzerland)  
El Kebir Hlil (Universite Joseph Fourier, Grenoble, France)  
Jana Houserová (Masaryk University, Brno, Czech Republic)  
Jonathan Keartland (University of the Witwatersrand, Johannesburg, South Africa)  
Jaime Keller (TU-WIEN, Austria)  
Jai Sam Kim (Pohang Univ of Science and Tech, Pohang, Korea)  
Jürgen Köhler (Max-Planck-Institut, Stuttgart, Germany)

Anton Kokalj (J. Stefan Institute, Ljubljana, Slovenia)  
Andrzej Kolezynski (University for Mining + Metallurgy, Krakw, Poland)  
Anjali Kshirsagar (University of Pune, India)  
Jan Kunes (Institute of Physics, AS CR, Praha, Czech Republic)  
Dieter Kvasnicka (TU Wien, Austria)  
Dominik Legut (Academy of Sciences, Brno, Czech Republic)  
Xiaogang Lu (Royal Institute of Technology, Stockholm, Sweden)  
Joachim Luitz (TU Wien, Austria)  
Georg Madsen (TU Wien, Austria)  
Maria Magnitskaia (Institute for High Pressure Physics, Moscow, Russia)  
Pavel Novak (Institute of Physics, Praha, Czech Republic)  
Torsten Ohm (Universität Dortmund, Germany)  
Emmanuelle Orhan (Universite de Rennes, France)  
J. Manuel Perez-Mato (Univ. Pais Vasco, Bilbao, Spain)  
Clas Persson (Uppsala University, Sweden)  
Mark Prandolini (Freie Universität Berlin, Germany)  
Franz Renz (Johannes Gutenberg-Universitaet Mainz, Germany)  
Juarez L.F. Da Silva (Fritz-Haber Institut MPG, Berlin, Germany)  
Karlheinz Schwarz (TU Wien, Austria)  
Andrew Scott (University of Leeds, United Kingdom)  
Vyacheslav Samokhvalov (TU Bergakademie Freiberg, Germany)  
Kentaro Uehara (National Research Council of Canada,Sussex,Canada)  
Roser Valenti (Universitaet des Saarlandes, Saarbrücken, Germany)  
Asta Storebo Villanger (Norwegian Defence Research Establishment, Kjeller, Norway)  
Frank Wagner (MPI fuer chemische Physik fester Stoffe. Dresden, Germany)  
Kerstin Weinmeier(TU Wien, Austria)  
Wolfgang Wenzel (Dortmund University, Dortmund, Germany)  
Marc Willinger (TU Wien, Austria)  
Lilia M. Woods (The University of Tennessee, Knoxville, USA)  
Guang Zheng (Dortmund University, Dortmund, Germany)

(Karlheinz Schwarz)

## 5 News from the ESF Programme

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

#### 5.1 Call for Workshop Proposals for 2001

It is not too early to consider proposals for Workshops to be held in 2001 for (partial) funding by the ESF Psi-k Programme.

Proposals should be submitted by email to the Psi-k Programme secretary, Walter Temmerman, at

psik-coord@dl.ac.uk

by August 31, 2000, and should include the following points.

1. Title and purpose of the Workshop, with names and addresses (incl. email) of the organisers.
2. The scientific content and why a workshop would be useful at this time.
3. A tentative list of speakers whom it is hoped to have.
4. The number of participants it is planned to invite or attract, and their scientific involvement, eg. as simulators, related experimentalists, code developers etc.
5. A budget and statement of other organisations which will be applied to for co-sponsorship and additional funding, eg. the TMR Network on Electronic Structure, the RTN Network on Magnetoelectronics, CECAM, CCP-9 in the UK, etc.. The support from the ESF Psi-k Programme has in the past been limited to 60k French Francs.
6. Where it is hoped the Workshop would be held.
7. The purpose of the ESF Psi-k Programme is to help everyone in our community to do good quality research. In order to achieve it some good people need extra know-how or new collaborations. Workshop organisers are asked to please consider how their programme and publicity might further this process in their field.

(Volker Heine, chairman of ESF Psi-k Programme)

## 5.2 Workshop Announcements

### 5.2.1 Workshop in Brighton, UK

## Extended Defects in Semiconductors

July 18-22, 2000, Brighton, UK

**Sponsors:** Psi-K/ESF, EU-Interreg Transdiam, British Carbon Group

**The Workshop's web site:**

**<http://www.cpes.susx.ac.uk/eds2000>**

The accent of the Workshop is on the link between modelling and experiment. We hope this is of some interest to you.

The list of confirmed invited speakers is:

Phil Batson (*IBM*),  
Paul Brown (*University of Nottingham, UK*),  
Mick Brown (*University of Cambridge, UK*),  
Anna Cavallini (*University of Bologna, Italy*),  
GBbor Csanyi (*MIT, US*),  
David Cherns (*University of Bristol, UK*),  
Jean-Luc Demenet (*University of Poitiers, France*),  
Victor Higgs (*Bio-Rad, UK*),  
Alain Jacques (*+cole de Mines, Nancy, France*),  
Vitaly Kveder (*Chernogolovka, Moscow, Russia*),  
Koji Maeda (*University of Tokyo, Japan*),  
Pat Mooney (*IBM*),  
John Northrup (*Xerox Palo Alto, US*),  
Ricardo Nunes (*UFMG, Brasil*),  
Sergio Pizzini (*University of Milan*),  
Fernando Ponce (*Arizona State University, US*),  
Jacques Rabier (*University of Poitiers, France*),  
Eric Stach (*Lawrence Livermore, US*),  
Takayoshi Suzuki (*University of Tokyo*),  
Guy Vanderschaeve (*CEMES, Toulouse, France*),

Jörg Weber (*TU Dresden, Germany*),  
Jan Weyher (*University of Nijmegen*),  
Peter Wilshaw (*University of Oxford, UK*)

## 5.3 Mid-term Report on ESF Psi-k (STRUC) Programme

January 1998 to April 2000

Web sites:

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

<http://www.esf.org/physical/pp/STRUCa.htm>

### 1. Scientific developments

#### 1.1 A brief outline of what we do

We are a community of researchers in computer simulation or computational physics that has grown and is growing exponentially from small beginnings towards the end of the 1970s. Everything that happens in any material at the atomic level is governed by the valence electrons in and between the atoms. These bond the material together and react to any external stimulus. This applies to everything from a biological molecule to magnetism to a chemical reaction at a catalytic surface. Previously the behaviour at the atomic level has been represented in computer simulations by some empirical bonding forces between atoms, expressed as classical interaction potentials. That is a good starting point, but not good enough for countless situations. There one has to do very large computations to solve the basic quantum mechanical equations for all the electrons in the given system. These are called 'ab initio' or 'first principles' simulations, and that is what our community does. They amount to 'computer experiments' to elucidate processes not directly accessible to laboratory experiment. Our methodology has application to various areas of physics, chemistry, materials science and recently other sciences (see 1.2 and 1.3 below).

#### 1.2 Recent developments in our field

Our field of research has continued to grow very dynamically. For example, the circulation of the Psi-k Newsletter (see item 4.3 below) has increased from about 500 in 1997 to 760 now. Some of these are for public display in substantial research groups, so that with the inclusion of research students the whole community in Europe must be between one and two thousand. Several hundred people have participated in the workshops to date, and over 500 suggestions were received for invited speakers for our big Psi-k2000 Conference (item 4.5).

There has been a very noticeable increase of the involvement of our community with industry, as described more fully in sect. 4.7 below. Here we pick out just one item, the establishment of an annual Catalysis Workshop bringing together regularly our community with experimentalists in catalysis and researchers from industry. Going with this has been a growing number of calculations involving the adsorption and dissociation of molecules on surfaces. While we do not want to exaggerate the total industrial impact of our methodology at present, one certainly sees a number of growth points and new initiatives.

There are many examples where one can see the gap closing between what our calculations can deliver and what experimentalists want, due both to cleverer computer codes and to growth in computing power. Three years ago the majority of calculations were static ones, representing materials at zero degrees Kelvin, but now calculations are routine which include the thermal agitation of the atoms at whatever temperature. Similarly whereas previously one could only calculate energy differences, one now often calculates the more relevant thermodynamic free energy including vibrational entropy.

One can see a broadening of the range of materials and processes being calculated. Until recently oxides were 'sometimes a bit difficult' but now there are calculations on the adhesion of a metal to an oxide, and the thermodynamics and detailed structure of the interface. Similarly simulating all the complex steps in crystal growth is now being achieved and the self-assembly of quantum dots on a surface.

The range of applications has widened, for example a doubling of the number of centres using our methodologies for studies in mineralogy. The application to biological processes is new, with one person we know of funded directly by the pharmaceutical industry.

There has been an impressive number of technical developments in our field, of which we mention just one. Svane and others have developed a method for taking into account the strong electron repulsions among electrons in the f-shell of rare earth and actinide elements, which goes beyond the local density approximation and gives a good account of their valence and bonding in metals and compounds containing these elements. Thus our methodology is being extended to cover all the elements in the periodic table, as needed by researchers in many fields, not just the elements that the theoreticians happen to find easy.

Some of the above points can be illustrated by reference to the latest issue (17.April,2000) of Physical Review Letters, the most prestigious journal in physics. Out of a total of 56 articles covering the whole of physics, 5 report calculations with our methodologies, which shows the importance of our field and its contribution to the front line of research. Of the 5 articles, two come from Europe, two from USA and one from Japan, demonstrating the important contribution of Europe. Its relevance is shown by the opening sentences of one of the articles (from Berlin) in a joint project with industry:- "The nature of the corundum surface (alpha aluminium oxide) is of considerable importance in a wide variety of technological applications. These range from catalytic supports and thin-film substrates to corrosion and wear protection in mechanical systems."

The contribution of our community to European science is also shown by the award of two specialised EU TMR Networks and recently one EU RTN Network under the new EU Framework.

### **1.3 One specific scientific highlight as an example**

The broad contribution of our methodology and the importance of European collaboration are well illustrated by the following scientific highlight from an interdisciplinary collaboration with earth scientists.

The core of the Earth consists mainly of liquid and solid iron which it is difficult to study in the laboratory at the simultaneously high temperatures and pressures. Professor M J Gillan and an international team of co-workers reported calculations [Nature 40, 462 (1999) and references there] on the free energies of the solid and molten forms and hence deduced the melting curve. The calculations were done in the UK with a computer code developed in Austria by G Kresse, and they involved G A de Wijs from the Netherlands, L Vocadlo from the Czech Republic, D Alfe from France as well as G D Price and J Brodholt from the UK. The work was commented on in Nature and reported in Britain on the main television news. The calculations are being extended to determine the solubilities of MgO and SiO<sub>2</sub> from the Earth's mantle in the iron core, which is relevant to several questions ranging from interpretation of earthquake travel times to the energetics sustaining the Earth's magnetic field.

## **2. Organisation and budget of Psi-k Programme**

### **2.1 Organisation**

There are now 17 countries participating in the Programme, which are listed in appendix 2.1.1 with the supporting ESF Member Organisations. We believe this is a larger number than in any other ESF Programme to date, reflecting the fact that we represent a substantial research community (see discussion in item 3 below). However the budget of about 900 kFF per year is modest.

Decisions are made by a Core Group of 20 members of the Steering Committee, one from each country (and two from Belgium!) plus two officers. This meets normally once per year, but is constantly in email contact to make minor decisions between meetings. For example we give ourselves a deadline of two weeks from submission to make a decision about an application for support for a short bilateral visit. The names of all the Steering Committee members are given in Appendix 2.1.2.

The whole Steering Committee consists of the above Core Group plus 14 other Advisory Members (also listed in Appendix 2.1.2) whose expertise is needed in view of the broad range of the Programme's activities. It is kept in touch with the Core Group by email, and has met once in person at the beginning of the Programme. All its members were also invited to the Programme Committee meeting for the big Psi-k2000 Conference at which invited speakers were chosen (see item 4.5 below).

The Psi-k Newsletter (item 4.3 below) is also very important in keeping everyone involved with the Programme in touch.

## 2.2 Budget

The budget for year 2000 and the accounts for 1998 and 1999 are given in Appendix 2.2. The annual expenditure is about 900 kFF.

## 3. Goals of the Psi-k Programme

In order to explain the goals of the Psi-k Programme it is necessary to enlarge on the nature of our work and our community.

The type of research has already been described in section 1.1 above. Such quantum mechanical calculations are voracious in their demand for computer power. Indeed to make the computations feasible at all, it is necessary to use every possible trick both in computational algorithms and in ways of representing the desired science in the computer. Thus although there is a common broad basis to all the work, there is no single computer code that does everything needed. There are several types of code for different types of application and each of these has further variations e.g. as between metals and insulators, magnetic and non-magnetic materials, heavy elements where relativistic effects are important etc. On the other hand the same basic code may be used in very different areas of science, e.g. surface chemistry and defects in semiconductors. We are therefore a very diffuse community scattered across various sciences, but using a broadly common methodology.

**Three broad goals become apparent from this picture.**

Goal One: *'Linking'*

There is an enormous need to link researchers using similar techniques in order to share new technical advances, to learn from each other what new ideas work and which ones do not (which usually does not get into the published literature). Peoples' primary connection is to the field of application with which they are concerned. This is as it should be: our community is characterised by close connection with experimentalists. But clearly the researchers also need close contact with others sharing a similar technique in this rapidly moving field. Whereas some experimental areas of research have some major facility as a natural meeting point, our community needs something quite different because our computations are done in-house on powerful workstations or by electronic link to some distant supercomputer which one never sees. Our community needs firstly a communication infra-structure, namely the Psi-k Newsletter and Psi-k Steering Committee etc., and secondly meetings of various types ranging from bilateral visits

through tutorial and research workshops to the conference in year 2000. These activities of the Psi-k Programme therefore provide the links between researchers. Before the EU Human Capital and Mobility Network and two small efforts which preceded the present ESF Programme there were almost no connections: no address list, no organisation, no series of workshops or conferences, no nothing.

Goal Two: *'Quality'*

Our second goal is promoting high quality in research. It has been said that second rate research is hardly worth doing. Another saying in computing is 'Garbage in, garbage out'. Our types of computations are very very sophisticated, and many tricks are needed to get the calculations into the available computers at all, even the largest ones, and controls to get reliable answers. With a rapidly expanding field, many of the researchers are relatively young and inexperienced, often in somewhat isolated small groups springing up in diverse institutes and universities. The activities of the Psi-k Programme therefore include training, sharing best techniques, and linking younger researchers to strong experienced groups. We think that largely as a result of such collaboration under the present ESF Programme and previous EU HCM Network, Europe is now the leading area in the world for our type of research, and we want to keep it that way.

Goal Three: *'Extension'*

Our third goal is to promote the extension of our methodology to new areas of science through special workshops, talks at conferences and other activities. We admit a bit of visionary zeal here, having seen the power of our methodology in existing fields.

The fact is that one European country is too small a unit to sustain research at the world forefront in this field. By vigorously promoting collaboration, the Psi-k Programme is enabling young people to do first class science.

## **4. Report on activities**

We will summarise the activities for the years 1998 and 1999, and those in the pipeline for 2000.

### **4.1 Hands-on tutorial training workshops**

These workshops run for one week, concentrating in the afternoons on practical use of a particular computer code. Mornings are devoted to lectures and exercises in the background theory to make intelligent and best use of the code. Before or after the evening meal the students on the course present for discussion their planned research topic. The students are mostly Ph.D.

students, with some more senior researchers wanting to get into the field.

Two tutorial workshops were held in 1999, with two planned for 2000, as listed in Appendix 4.1. Reports and further details can be found in the on-line copies of the Psi-k Newsletter at the psi-k web-site given at the top of this report.

They further the goals 'Linking' and 'Quality' (sect. 3).

## **4.2 Research workshops**

These are the main avenue for the sharing of experience and expertise among researchers, i.e. serving the goals 'Linking' and 'Quality'(sect. 3). A strong series of workshops covering a wide spectrum of topics has been held and planned in 1998 to 2000 as listed in Appendix 4.2. There is a report on each Workshop in the Psi-k Newsletter which can be accessed as detailed in Appendix 4.2.

Some of these workshops also serve the goal 'Extension' by focussing on the very fringe of what has been done in the past or purposely discussing what can be done in a new direction, or bringing in experimentalists or others from a different discipline, e.g. at the 'industry' workshop in 1998 or the workshop on materials at high pressures in 1999.

## **4.3 The Psi-k Newsletter**

The Newsletter is a great success and important in creating a community, i.e. serving mostly the 'Linking' goal of sect. 3. Its email address list of 760 names now has become the main vehicle for advertising jobs and announcing conferences from other organisations likely to be of interest to our community, e.g. the Euresco conferences related to electronic structure calculation on solids. Such items are inserted in the Newsletter but also circulated separately, especially in the time gap between successive issues.

The Newsletter appears every two months, distributed by email and posted on the web site. It has from 50 to 100 pages, and includes the activities of the two EU TMR Networks in our community. A report appears from every workshop and bilateral visit or other activity funded by the Programme. There is a 'highlight' article on some particularly successful or important piece of research, thus serving the 'Quality' goal of sect.3. Any researcher can submit a one-page abstract of any new paper sent to a journal for publication, with an email address for contacting the author(s).

The current issue and all past issues of the Newsletter may be consulted and down-loaded from the psi-k web-site given at the head of the report.

## **4.4 Bilateral visits**

These short visits (listed in Appendix 4.4) of a few days or at most a few weeks are extremely valuable, and serve the goals 'Linking' and 'Quality' of item 3. They are especially valuable to researchers in isolated groups when needing to draw on the expertise of a more experienced group. Most of the visitors are young researchers (and a good proportion appear to be women). Although this had been a very successful part of the programme of the earlier EU HCM Network, the up-take was unfortunately rather slow at first in the present ESF Programme. On inquiry it was found that people were very confused between the earlier EU HCM Network, the new EU TMR2 Network (item 5.1) and the present ESF Programme, and they don't know whether they belong and can apply. This is part of the problem with the short-termism of EU (and ESF) funding. The scheme of bilateral visits was therefore readvertised, and the up-take has become much better.

Each visit is different and serves some different research need, as shown by the list of topics in Appendix 4.4. It is particularly useful that the funding can be approved quickly when needed. Sometimes the visit is to a collaborating group of experimentalists to discuss the results of a calculation or some new experimental input. Often the purpose is to learn about some particular new computational development or piece of expertise. Sometimes a new young researcher needs training in the use of a particular computer code. Research groups working on closely related topics need to have in-depth discussion of their research plans so as to avoid duplication and to benefit from each others insights.

#### **4.5 The big Psi-k2000 conference**

The big conference in August 2000 covering the whole of our field will be the second such gathering in the world, the first one having been organised by us under the EU HCM Network in 1996.

Four plenary speakers and over 100 invited speakers (with 9 from industry) have been arranged, chosen from over 500 suggestions received from our community. They will be grouped in 19 Symposia covering the whole field. There will be 130 short contributed oral papers and an unlimited number of slots for poster presentation.

More details are given on the special web site:

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

#### **4.6 Euresco conferences**

Of course these are not directly under our auspices but there has been one conference almost every year under the broad heading of electronic structure of solids. These further all our three goals above so that they lie close to our heart. We therefore put some money into the 1998 and 1999 conferences to enable them to take place at all: details are given in Appendix 4.6. In fact all the past chairmen of these conferences are active in our Programme. How the conferences

further our goals 'Linking' and 'Quality' is obvious, but they also further the goal 'Extension' by mixing experimentalists and computationalists and theoreticians to show where computations would be useful. The conference proposed for 2002 will be the first in the world to focus on the contribution of our type of computation to biology.

#### **4.7 Links with industry**

We regard the links with industry as very important as part of our goal 'Extension' (sect. 3), though we do not want to exaggerate the impact of our methodology at the present time. One of our Steering Committee members Dr E Wimmer has recently set up his own company, spun off from Molecular Simulations Inc in Paris, to do calculations for industry. Another Steering Committee member Prof Norskov is joint holder of a patent for a new catalyst which could not have been developed without his calculations. Three more of our Steering Committee members (Hafner, Scheffler and Nieminen) also have long-term collaborations with industry, as do several others in our community. There are certainly several dozen copies of codes using our methodology that have been sold or licensed to industry.

A special 'industry' workshop was held in 1998 to bring together industrial researchers and ourselves. This has developed into an annual Catalysis Workshop as a regular meeting place for our community with experimentalists and researchers in industry: see the list of workshops for 1998, 1999 and 2000 in Appendix 4.2. There are 9 invited speakers from industry on the programme for the 'Psi-k 2000' conference (sect. 4.5).

There is therefore no doubt that our research is contributing to basic understanding of topics of industrial interest and to pre-competitive industrial research, and occasionally to solving a real industrial problem. Examples include calculations on cytochrome P450 enzyme funded by Glaxo Wellcome, bonding at metal/oxide interfaces, catalysis, defects in semiconductors, magnetic multi-layers for recording, transistor behaviour of conducting polymers, and development of a new pigment.

A joint hands-on tutorial training workshop is currently being planned with the Cambridge branch of the company MSI.

Apart from these organisational links, there are a number of personal contacts through our individual members.

#### **4.8 The working groups**

The original application to ESF envisaged a large number of Working Groups organising collaborations across the whole range of our activities. Such Working Groups were a successful part of the organisation and activity of the earlier EU HCM Network. However only some of the present Working Groups are really working, mostly those also in the EU TMR2 Network (item 5.1) and the EU TMR1 Network (item 5.2). We have analysed the reasons for this change, which

is largely due to being victims of our own success and our management structure not adapting to our growth. This matter is now being addressed and an effort being made to stimulate more Working Groups into action.

## **5. Relations with other European organisations**

Collaboration with other organisations mostly concerns joint funding of workshops and other activities, with other mutual support, as follows.

### **5.1 EU TMR Network 'Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Science' referred to as TMR2**

The scientific goals of this Network overlap considerably those of the Psi-k Programme, but of course the rules of EU TMR Networks are very different so that the two organisations are mutually complementary. In particular, the EU Network is very restricted in the number of groups and hence in the number of people it can reach, whereas the the activities of the Psi-k Programme are open to all workers in the field in Europe. Some workshops have been run jointly, and the Network contributes to the cost of the Newsletter and the Psi-k2000 Conference. A main goal of the Network is to establish links with industry, and the Psi-k Programme participates in this.

### **5.2 EU TMR Network 'Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers' referred to as TMR1**

This specialised and restricted network is a spin-off from the earlier general EU HCM Network. A few workshops have been jointly organised and funded, and the Network contributes to the Psi-k Newsletter (item 4.3), the Psi-k2000 Conference (item 4.5) and the links with industry (item 4.7).

### **5.3 Industry**

This has been covered in Section 4.7 above.

### **5.4 Centre Europeen de Calcul Atomique et Moleculaire (CECAM)**

There have been several jointly funded workshops. The location and infra-structure of CECAM in Lyon are indeed very convenient, their publicity particularly in the chemistry world serves our 'Extension' goal (sect. 3), and joint funding supplements our resources. Four of the workshops planned for year 2000 will be jointly organised and funded.

### **5.5 ESF Programme SIMU**

Mostly our activities are complementary, but there are some points of overlap on which we are trying to develop collaboration. One of the workshops this year will be jointly funded and advertised.

### **5.6 Trieste Total Energy and Force Workshops**

These are small conferences every two years and smaller workshops in the years in between, surveying the latest developments more or less across our whole field. Of the latter, the one in Spain in 2000 is being jointly funded, but otherwise the 'Trieste Workshops' have been financially independent.

### **5.7 ESF Euresco Conferences**

This has already been discussed in item 4.6.

## **6. The future**

The present ESF Programme is exactly the help that our community needs in pursuing research on a European basis, except for one major thing, namely that the Programme disappears after 5 years and we understand cannot be renewed. Everybody on the European scene (including ESF) likes to start new schemes but not to continue successes. Our community needs an on-going infra-structure reviewed and renewable periodically. Computing and computer simulation are not going to go away: on the contrary, we are still at the beginning of what will be a growth point for years to come. It is not a large sum of money for a community of our size.

Since there seems to be zero opportunity to achieve a continuing basis in the foreseeable future, we are discussing what temporary provision we might be able to make from the end of the present ESF Programme.

## APPENDICES

Note: the appendices are numbered according to the sections in the main report to which they relate.

### **Appendix 2.1.1:** Countries and ESF Member Organisations supporting the Psi-k Programme

Austria, Belgium, Czech Republic, Denmark, Finland, France, Germany, Hungary, Ireland, Italy, Poland, Portugal, Slovenia, Spain, Sweden, Switzerland, United Kingdom.

### **Appendix 2.1.2:** Members of the Steering Committee

The committee consists of the following Ordinary Members: Belgium: Vic Van Doren (Flemish Community) and Jean-Pol Vigneron (French Community), Denmark: Axel Svane, Finland: Risto Nieminen, France: Hugues Dreyse, Germany: Stefan Blugel, Hungary: Janus Kollar, Ireland: Charles Patterson, Italy: Raffaele Resta, Poland: Adam Kiejna, Portugal: Jose-Luis Martins, Slovenia: Ales Zupan, Sweden: Olle Eriksson, Switzerland: Rene Monnier, UK: Mike Finnis. The Chairman is Volker Heine, the Acting Chairman is Juergen Hafner and the Secretary is Walter Temmerman.

### **Appendix 2.2:** Summary of accounts for 1998 to 2000

#### *Summary of accounts for 1998*

Income (Contributions from Member Organisations): 847,200.00

Expenditure 497,285.48

Total balance (to be brought forward) 349,914.52

#### *Summary of accounts for 1999*

Income:

Contributions from Member Organisations: 899,200.00

Balance carried forward:

- for grants: 6,200.00

- for general purposes: 343,714.52

Total: 1,249,114.52

Expenditure:

Total expenditure: 674,323.75

Balance carried forward:

- for psi-k2000 Conference: 120,000.00

- for grants: 14,539.11

- for general purposes: 440,251.66

Total: 1,249,114.52

*Budget for 2000*

Income:

Contributions from Member Organisations: 899,200.00

Balance carried forward:

- for psi-k2000 conference: 120,000;00

- for grants: 14,539.11

- for general purposes: 440,251.66

Total: 1,288,699.11

#### **Appendix 4.1:** Hands-on tutorial training workshops

Detailed reports are contained in the Psi-k Newsletter which may be accessed from the Psi-k website given at the top of the report.

1. Full-potential LAPW calculations with the WIEN97 code, 7 - 10 April 1999 at TU Wien, Austria. Organised by P Blaha and K Schwarz, jointly sponsored with the Technical University of Vienna.
2. Calculation of materials properties using energy and force methods and ab-initio Molecular Dynamics, 9 - 19 August 1999 at ICTP, Trieste, Italy. Organised by P Kratzer, J Kohanoff, J Neugebauer and M Scheffler, jointly sponsored with EU TMR Network 'Electronic Structure'.
3. Hands-on tutorial course on use of the new LAPW code, organised by S Bluegel. Summer 2000.
4. Hands-on tutorial course on the CASTEP pseudopotential and plane wave code, at Dares-

bury, organised by V Milman, W Temmerman and others. Autumn 2000. Jointly sponsored with Molecular Simulations Inc.

Note: The workshops 'Computational materials science' held in Sardinia in 1998, 1999 and 2000, and 'Interface anisotropy and spin and orbital magnetism' held in Sweden in 1999, all listed as research workshops in Appendix 4.2, are also largely of a tutorial nature in the background theory in an active area of research.

#### **Appendix 4.2: Research workshops**

Detailed reports may be found in issues of the Psi-k Newsletter which can be accessed via the Psi-k website given at the top of the report.

##### **1998 (6 research workshops)**

1. Electronic structure calculations for industry and basic sciences. Vienna 3-4 June 1998. Organised by J Hafner, W Temmermann, E Wimmer and A Svane, co-organised with EU TMR Network "Electronic Structure".
2. Local orbitals for large scale atomistic simulations. Lyon 22-25 July 1998. Organised by D Pettifor, P Ordejon, L Seijo and G Galli, co-organised with CECAM.
3. Computational materials science. Santa Margarita, Sardinia 18-22 Sept 1998. Organised by P Ruggerone and V Fiorentini, co-organised with Univ. of Cagliari.
4. Properties of inorganic crystals from theory and experiment. Ploen 26 Sept-1 Oct 1998. Organised by B Winkler, K Knorr and V Milman, co-organised with Deutsche Ges. f. Kristallogr. and MSI.
5. Tight-binding LMTO method. Ste Odile 2-5 Oct 1998. Organised by H Dreysse, co-organised with EU TMR Network "Interface Magnetism".
6. Materials under high pressure: from ices to metals. Daresbury Lab 17-18 Dec 1998. Organised by W Temmermann, co-organised by EU TMR Network "Electronic Structure" and UK EPSRC CCP-9.

##### **1999 (7 research workshops)**

1. Hydrogen in semiconductors. U Exeter 14-17 April 1999. Organised by R Jones, co-organised with UK EPSRC CCP-9.
2. Interface anisotropy and spin and orbital magnetism. Riksgransen 5-9 May 1999. Organised by L Nordstrom, J Henk and O Eriksson, co-organised with Swedish NFR and Swedish KVA.

3. Catalysis from first principles. Magelas, DK, 17-19 May 1999. Organised by J Norskov, M Scheffler and J Hafner, co-organised with EU TMR Network "Electronic Structure".
4. Progress in materials science. Strasbourg 1-4 June 1999. Organised by H Dreyse and L T Wille, co-organised with E-MRS.
5. Orbital and spin magnetism of actinides. Daresbury Lab 4-5 June 1999. Organised by W Temmermann and G van der Laan, co-organised with EU TMR Network "Electronic Structure".
6. Calculation of electronic excitations in finite and infinite systems. Lyon 31 Aug-3 Sept 1999. Organised by L Reining, G Onida and A Rubio, co-organised with CECAM.
7. Computational materials science. Villasimius, Sardinia 10-13 Sept 1999. Organised by V Fiorentini and P Ruggerone, co-organised with Regione Autonoma Sardegna and UNESCO.

#### **2000 (9 research workshops)**

1. Advances in first-principles computational condensed matter physics. Madrid 13-15 Jan 2000. Organised by E Artacho, A Garcia and P Ordejon, co-organised with Trieste 'Total Energy and Force Workshops', Univ Auton Madrid, Univ Pais Vasco, Spanish CSIC and Motorola.
2. The fifth European workshop on solving the Bogoliubov de Gennes equations. Bristol Univ 14-16 April 2000. Organised by J Annett, K P Duncan, B Gyorffy and E Gross, co-organised with EU TMR Network 'Electronic Structure' and UK EPSRC CCP-9.
3. Electronic and optical properties of semiconducting glasses. Lyon 13-16 June 2000. Organised by D Drabbold, G Barkema, N Mousseau and P Ordejon, co-organised with CECAM.
4. Catalysis from first principles. Lyon 5-8 July 2000. Organised by M Scheffler, J Norskov and J Hafner, co-organised by EU TMR Network 'Electronic Structure' and CECAM.
5. Extended defects in semiconductors. Univ Sussex 18-22 July 2000. Organised by M Heggie.
6. Excited states and electronic spectra. Lyon 20-22 July 2000. Organised by L Reining, G Onida and A Rubio, co-organised with CECAM.
7. Across the length scales II: applications (MML2000). Oxford July 2000. Organised by D Pettifor, A Sutton R Rudd and S Kenny, co-organised with ESF Programme SIMU.
8. Workshop on computational materials science. Villasimius, Sardinia 8-11 Sept 2000. Organised by V Fiorentini, P Ruggerone, F Meloni and A Baldereschi, co-organised with Univ Cagliari, INFN and UNESCO.

9. Future developments in the study of structure-property relations by computational crystallography and experiments. Lyon 23-27 Oct 2000. Organised by B Winkler and V Milman, co-organised with CECAM.

#### **Appendix 4.4: Bilateral visits**

Details of each visit can be found in issues of the Psi-k Newsletter which may be accessed through the Psi-k website given at the head of the report.

#### **1998 (9 visits)**

1. A Lichtenstein (FZ Juelich, D) to K Kunc (U Paris VI, F), 5 days,  
*Electronic structure and lattice of manganite perovskite*
2. A Postnikov (U Osnabrueck, D) to M Alouani (U Strasbourg, F), 5 days,  
*Metal/insulator transition in RENO3 perovskites*
3. E Wachowicz (U Wroclaw, PL) to C Stampfl (FHI Berlin, D), 14 days,  
*Electronic and structural properties of hcp metals and surfaces*
4. R Kucharczyk (U Wraclaw, PL) to J Pollmann (U Muenster, D), 28 days,  
*Interfaces and superlattices of semiconductors*
5. S Razee (U Warwick, UK) to L Szunyogh (CMS Wien, A), 12 days,  
*Magnetic anisotropy of thin films and multilayers*
6. A Zupan (U Ljubljana, SL) to P Blaha (TU Wien, A), 5 days,  
*Exchange-correlation functionals*
7. R Schmidt (U Frankfurt/M., D) to K Schwarz (TU Wien, A), 5 days,  
*Relativistic local orbitals in FLAPW*
8. W Hofer (CMS Wien, A) to S. Bluegel (FZ Juelich, D), 2 days,  
*Scanning tunneling microscopy simulations*
9. K Kadas (TU Budapest, H) to J Hafner (CMS Wien, A), 28 days,  
*Reconstruction of BN surfaces*

#### **1999 ( 13 visits)**

1. C Filippi (Univ. Coll. Cork, IRL) to M Scheffler (FHI Berlin, D), 5 days,  
*Hydrogen on Si(100) using Quantum Monte Carlo*
2. C Molteni (U Cambridge, UK) to M Parrinello (MPI Stuttgart, D), 8 days,  
*Phase transformations in nanocrystals; photoreactions*

3. B Ujfalussy (U Budapest, H) to B Gyorffy (U Bristol, UK), 8 days,  
*Quantum wires; oscillatory exchange coupling; domain walls*
4. M Miao (U Antwerp, B) to J L Martins (U Lisbon, P), 8 days,  
*Pseudopotential codes; GGA implementation*
5. D Koedderitzsch (U Halle/Saale, D) to W Temmerman (Daresbury Lab., UK), 25 days,  
*Electronic structure of transition metal oxides*
6. E Sjoestedt (U Uppsala, S) to M Scheffler (FHI Berlin, D), 4 days,  
*Training on FLAPW and FHI98 codes*
7. R Grohmann (U Wien, A) to S Bluegel (FZ Juelich, D), 5 days,  
*Cerium oxide surfaces; FLEUR code development*
8. T Korhonen (TU Helsinki, SF) to S Bluegel (FZ Juelich, D), 5 days,  
*FLEUR code development*
9. S Shallcross (U Bristol, UK) to I Abrikosov (U Uppsala, S), 90 days  
*Compositional order and disorder at alloy surfaces*
10. A. Taga (U Uppsala, S) to C. Ambrosch-Draxl (U Graz, A), 9 days,  
*Implementing electron-phonon coupling in LAPW*
11. R. Grohmann (U Wien, A) to S. Bluegel (FZ Juelich, D), 7 days,  
*Training in local orbital extension of FLEUR code*
12. C Rovira (U Barcelona, E) to M. Parrinello (MPI Stuttgart, D), 14 days,  
*Coenzyme and hemeprotein dynamics*
13. G. Madsen (U Aarhus, DK) to K. Schwarz (TU Wien, A), 22 days,  
*Non-nuclear maxima of electron density*

**2000 with reports received by 1 April Newsletter (4 visits)**

1. P. Korzhavi (U. Uppsala, S) to R. Podloucky (U Wien, A), 6 days,  
*Planning collaborations on defects in intermetallics*
2. J.L. Mozos (TU Helsinki, SF) to E.K.U. Gross (U Wuerzburg, D), 19 days,  
*Time-dependent DFT for excitations in insulators*
3. D. Koedderitzsch (U Halle, D) to W. Temmerman (Daresbury Lab, UK), 12 days,  
*Self-interaction corrections in transition metal oxides*
4. P. Ghosez (U Liege, B) to P. Ordejon (CSIC Barcelona, E), 4 days,  
*Planning collaboration on ferroelectric thin films*

**Appendix 4.6:** Euresco Conferences supported financially by the Psi-k Programme

1. Computational Physics for Nano-technologies, 19 - 24 September, 1998 at Il Ciocco, Italy. Organised by A Fisher
2. Challenges in the Predictive Description of Reaction Dynamics and Growth Properties of Surfaces, 18 - 23 September, 1999 at Leggries, Germany. Organised by A Gross, G Pacchioni and Th Kluener

Detailed reports can be found in issues of the Psi-k Newsletter which can be accessed through the Psi-k website given at the top of the report.

## 5.4 Reports on Collaborative Visits

### Report on a Collaborative Visit of Carla Molteni (Theory of Condensed Matter group, University of Cambridge) to the Max-Planck-Institut für Festkörperforschung, Stuttgart

26 March–2 April 2000

I visited Prof. Michele Parrinello and his group at the Max-Planck-Institut für Festkörperforschung in Stuttgart (Germany) from 26 March to 2 April 2000.

The aim of my visit was to discuss recent results and future developments of on-going collaborations on structural phase transformations in nanocrystals and photoreactions in proteins.

The visit has also benefited from the presence, at the same time, of Dr Roman Martonak from the Slovak Technical University of Bratislava (nanocrystal project), and Dr Irmgard Frank from the University of Munich (photoreactions).

Recently, we have developed a new constant pressure molecular dynamics method suitable for studying, within a density functional theory (DFT) scheme, non-periodic systems under pressure, which cannot be simulated with the usual techniques for periodic systems. The method consists in immersing a DFT treated non-periodic object 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 [R. Martonak, C. Molteni and M. Parrinello, *Phys. Rev. Lett.* **84**, 682 (2000), “*Ab-initio molecular dynamics with a classical pressure reservoir: simulation of pressure-induced amorphization in a  $Si_{35}H_{36}$  cluster*”].

We are presently extending the investigation to larger clusters of silicon, through the implementation of the the method within a tight-binding scheme: this allows us to treat many atoms for a longer time scale. Moreover, we are planning applications to other materials that has been experimentally studied.

We have also discussed some recent calculations on chromophores of photoactive proteins. A first study on this subject has been published in C. Molteni, I. Frank and M. Parrinello, “*An excited state density functional theory study of the rhodopsin chromophore*”, *J. Am. Chem. Soc.* **121**, 12177 (1999).

The visit has been very useful to discuss new ideas for future calculations and outline a couple of publications with the most recent results.

I am very grateful to the network for its support.

Carla Molteni

Cavendish Laboratory, Cambridge

**Report on a visit of Dr László Szunyogh (Budapest, Hungary) to  
Professor Balázs L. Györffy (Bristol, UK) and  
Dr Julie B. Staunton (Warwick, UK)  
April 3 - 15, 2000**

In the first ten days of my staying in UK I was visiting Prof Györffy's group at the Physics Department of the University of Bristol. The work we had before was to look over the results of the *first-principles calculations on a 90° Bloch Wall in BCC iron* and to complete a joint publication on it. The calculations were done before in Bristol by Jürgen Schwitalla by extending the spin-polarized relativistic Screened KRR code to the problem of a Bloch Wall and implementing it to the Cray machine in Manchester. By crossing the length-scale gap between atomic scales and the width of a Bloch-Wall, the Bloch-Wall energies almost up to 900 atomic layers were calculated in terms of the frozen potential approximation. An excellent agreement was found to most of predictions of the Landau-Ginzburg phenomenological theory. Preliminary self-consistent calculations, however, showed distinct variations of the electronic structure and the magnetic moments across the Bloch Wall. Through detailed discussions with Professor Györffy we completed the major part of the manuscript, which is now merely a subject of some final revisions. We also exchanged ideas on future progress of our first-principles investigations of Bloch Wall properties, which include self-consistent calculations of the Bloch Wall in terms of constrained Density Functional Theory, the study of (pinning) effects of impurities and lattice distortions to the Bloch Walls and also calculations of electronic transport across Bloch Walls.

In the next three days I visited Dr Julie B. Staunton at the Physics Department of Warwick University. Our common research project concerns the *magnetism of thin films at finite-temperatures* investigated within a mean-field disordered local moment picture. We discussed the formalism in conjunction to systems with 2D translational invariance, its possible extension to the relativistic case and also made progress in the Screened KKR code to calculate the paramagnetic spin-susceptibility. In the near future we are going to report on our calculations of the Curie temperatures in various thin-film systems, like Fe/W(001), Fe/Cu(001) and Co/Cu(001).

Dr László Szunyogh

Technical University Budapest, Hungary, April 19, 2000

**Report by Sorcha Healy (National University of Ireland, Cork)  
on a collaborative visit to the Fritz Haber Institute,  
Berlin (Apr 25–May 5 2000).**

As a PhD student at the National University of Ireland, Cork, I am currently studying the adsorption/desorption mechanisms of molecular hydrogen on the Si(100) surface. I intend to perform quantum Monte Carlo calculations of the reaction barriers of molecular hydrogen on the silicon surface and settle the long standing issue of the nature of the desorption mechanism.

In the last few months, I have been learning how to use existing quantum chemistry packages and have interfaced them with our quantum Monte Carlo (QMC) codes. This is a necessary step for the construction of the correlated wave functions which we will use in QMC to investigate the H<sub>2</sub>/Si(100) system. After several preliminary tests, we are now ready to attack the real problem of the hydrogen on silicon surface.

In order to implement this project several technical details needed to be discussed with Prof Scheffler's group in Berlin. These included the structure and geometry of the silicon cluster to be used, the pseudopotential for the silicon atom and the appropriate DFT functionals to use in determining the surface geometry. Also other mechanisms for the adsorption/desorption of molecular hydrogen had been investigated over the last year within the group in Berlin and these new clusters were taken into consideration in our discussions. A consensus was reached within the group on the order and priority of clusters to be studied and the above technical data.

As a secondary purpose to my visit, I discussed with several other researchers the nature of their work, the different surfaces and the methods which they use. Also there were some seminars which I attended , one on STM on transition metal surfaces. This was instructive as STM is one of the primary experimental tools in this area.

In conclusion, my visit to the Fritz Haber Institute both aided my immediate research and broadened my view of the work and uses of the surface science area.

Sorcha Healy

## 6 General Workshop/Conference Announcements

### 6.1 4th EPSRC/IOP Matter Summer School

#### 4th EPSRC/IOP Theory of Condensed Matter Summer School Ambleside, Cumbria, UK 3-15 September 2000 <http://www.bath.ac.uk/Physics/Summer>

The aim of the School is to teach material underpinning research in modern condensed matter theory, introducing concepts, techniques and problems that are the subject of current research in the field, illustrated with a wide range of applications. The School is directed towards post-graduate students in condensed matter theory, and theory-inclined students in experimental condensed matter physics, typically in their first or second year of research. The lecture courses will be presented by active members of the community, and accompanied by example classes with full tutorial support. A series of specialist seminars will highlight current research and applications.

The School, the fourth in a successful series, will be held in Ambleside, Cumbria, on the shores of Lake Windermere in the heart of the beautiful Lake District National Park.

The School is organised by the UK Institute of Physics Theory of Condensed Matter Group, and sponsored by the UK Engineering and Physical Sciences. The school fee is GBP650, including meals and accommodation.

#### **Lecturers:**

Dr James Annett (Bristol)	Superconductivity
Dr Simon Crampin (Bath)	Electronic structure
Prof Peter King (Imperial)	Applications of statistical physics
Dr Boris Mouzykantskii (Warwick)	Mesoscopics
Prof Philip Russell (Bath)	Photonics
Dr Andrew Schofield (Birmingham)	Strongly correlated systems
Dr Patrick Warren (Unilever)	Soft condensed matter
Dr Julia Yeomans (Oxford)	Statistical physics

Further details (including a registration form to download) may be found at the summer school web site: <http://www.bath.ac.uk/Physics/Summer> - alternatively, contact the organiser at the address below.

School organiser:

Dr S Crampin,

Department of Physics,

University of Bath, Bath, BA2 7AY, UK

email: [s.crampin@bath.ac.uk](mailto:s.crampin@bath.ac.uk)

Tel : +44 (0)1225 826826

Fax : +44 (0)1225 826110

## 6.2 UK Condensed Matter Theory Meeting

June 7, 2000, Warwick University, UK

Below is the programme for the annual UK Condensed Matter Theory Meeting, organised this year at Warwick University, under the auspices of the Institute of Physics.

Full details can be found at: <http://www.phys.warwick.ac.uk/theory>

### Programme of the meeting

- 10:30 Registration and Coffee
- 11:00 Dr David Cobden (Warwick)  
*"Nanotubes"*
- 11:45 Prof David Pettifor (Oxford)  
*"Bond-order Potentials: bridging the electronic to atomistic modelling hierarchies"*
- 12:30 Lunch
- 13:45 AGM of IoP Condensed Matter Theory Group
- 14:00 Dr Mark Warner (Cambridge)  
*"Chiral Imprinting"*
- 14:45 Posters with tea at 15:30
- 16:00 Prof Duncan Haldane (Princeton)  
*"Stripes in the Quantum Hall Effect"*
- 16:45 Close

Robin Ball, Boris Muzykantskii

## 7 General Job Announcements

### Two Ph. D. Positions in Condensed Matter Theory

#### Max-Planck-Institute Halle

The Max-Planck-Institute of Microstructure Physics at Halle, Germany, expects to have two **positions for Ph. D. students in Condensed Matter Theory** available for up to three years starting July 1, 2000. The candidates for these position will develop a many-body theory of **Femtosecond Spin-Dynamics** at antiferromagnetic oxide interfaces using non-perturbative methods. The theory envisages the laser control of magnetism, in particular antiferromagnetism, by nonlinear optics. This subject is closely related to the emerging technology of ultrafast spin-dynamics devices. Experience with many-body techniques (exact diagonalization, quantum chemical methods, Green's function techniques, and/or supersymmetry) or optical control formalisms is desired for these positions. The Max-Planck Society is an Affirmative Action/Equal Opportunity employer. Applications from women, minorities, and disabled persons are encouraged.

Candidates for the positions, which are open to all nationalities, must hold a Master's (or equivalent) degree and should send an application including a CV including the names of two references to:

Dr. W. Hübner,  
Max-Planck-Institut für Mikrostrukturphysik Halle,  
Weinberg 2, D – 06120 Halle,  
Fax: +49-345-5511 223,  
email:huebner@mpi-halle.de

**Ph. D. Position**  
**Physics Department, University of Muenster, Germany**

A PhD-Position is available in the research group of Prof. J. Pollmann in the Physics Department at the University of Muenster, Germany. The focus of the work will be on ab-initio calculations of structural and vibronic properties of semiconductor surfaces. The method is the density functional perturbation theory. Calculations will partially be done at the parallel computer at the Computer Center of the University of Karlsruhe. Applicants are expected to have some knowledge in applying numerical methods to physical problems, especially in conjunction with electronic structure theory. The salary is according to the german BAT IIa/2, which will be about 40000DM before taxes.

Applications should be sent to:

Prof. Dr. Johannes Pollmann  
Institut fuer Festkoerpertheorie  
Wilhelm-Klemm-Str. 10  
D-48149 Muenster  
Germany

or via e-mail: [pollman@uni-muenster.de](mailto:pollman@uni-muenster.de)

Futher information can be obtained contacting:

Dr. Albert Mazur at the same address or via e-mail: [mazur@uni-muenster.de](mailto:mazur@uni-muenster.de)

## **Post-doctoral Position**

### **Physics Department, University of Muenster, Germany**

A post-doctoral position in condensed-matter theory will be available at the Physics Department of the University of Muenster, in the group of Prof. Dr. J. Pollmann. The main focus of the project is on analytical and computational investigations of electronically excited states of molecules adsorbed at surfaces. In this context, the interaction of a molecule with the substrate, the coupling of its excitations to those of the substrate, and the dynamics of the molecule in the excited state are of particular interest. This will be described by highly reliable ab-initio techniques, i.e. by GW quasiparticle calculations followed by a determination of coupled electron-hole excitations. These approaches, which explicitly include electronic correlation effects, are based on preceding density-functional calculations.

The project is part of a focused program ("Electron transfer processes at interfaces") of the Deutsche Forschungsgemeinschaft (DFG). The position is for two years, with possible extension to up to four years. The salary will be about DM 70,000-80,000 before tax, depending on age and marital status.

The ideal candidate should have a PhD in physics, chemistry, or materials science. A strong background in computational physics, density-functional theory, and electronic correlation is desirable.

For further details, please contact (e-mail preferred):

Dr. Michael Rohlfing  
Institut fuer Theoretische Physik II  
University of Muenster  
Wilhelm-Klemm-Strasse 10  
48149 Muenster  
Germany

e-mail: [rohlfm@uni-muenster.de](mailto:rohlfm@uni-muenster.de)

Phone: +49 251 83-33584

Fax: +49 251 83-33669

homepage: <http://www.uni-muenster.de/Physik/TPII/Pollmann/tgo.htm>

Applications should be sent to:

Prof. Dr. Johannes Pollmann  
Institut fuer Theoretische Physik II

University of Muenster  
Wilhelm-Klemm-Strasse 10  
48149 Muenster  
Germany

e-mail: pollman@uni-muenster.de

Phone: +49 251 83-36311

Fax: +49 251 83-33669

## **Post-Doctoral Position in Electronic Structure Theory Cork, Ireland**

A postdoctoral research position (1 year, renewable for a second year) is available in the Electronic Structure Theory group in the Physics Department at University College Cork, IRELAND. The current research interests of the group are in the development and application of quantum Monte Carlo methods and, in collaboration with the materials modelling group at the National Microelectronic Research Centre, the investigation of electronic structure in nanoscale systems. Salary in the range 19-21,000 Irish pounds/annum.

Please contact:

Prof. Stephen Fahy,  
Department of Physics,  
University College Cork,  
IRELAND  
e-mail: s.fahy@ucc.ie  
Tel: +353-21-490-2452

**Post-doctoral Position**  
**Computer Modelling of Interfaces in Functional Ceramics**  
**Department of Materials Science and Metallurgy, Cambridge**  
**University**

Applications are invited for the above post funded by EPSRC to work with Dr P D Bristowe in the Atomistic Simulation Group at Cambridge University. The successful candidate will undertake first principles calculations on the atomic and electronic structure of doped grain boundaries in various electroceramic oxides including strontium titanate and titanium dioxide. The aim is to determine the role of interfacial segregation in controlling the functionality of device materials. The work will be closely coupled to a parallel experimental investigation of the properties of oxide grain boundaries using a range of analytical electron microscopy and spectroscopy techniques.

A Ph.D. in a relevant area of materials modelling, theoretical physics or chemistry is required and experience using electronic structure codes and atomistic simulation codes is highly desirable. The Atomistic Simulation Group is a member of the U.K. Car-Parrinello Consortium which uses and develops the CASTEP code on the CSAR Cray T3E computer at Manchester University. Further details about the group are available at <http://www.msm.cam.ac.uk/asg/>

The appointment is for 3 years commencing 1 October 2000. The starting salary is in the range 16,286 to 18,185 GBP (pay award pending). The closing date for applications is 16 June 2000.

Please mail or email your resume and names of three references to

Dr P D Bristowe,  
Department of Materials Science and Metallurgy,  
Cambridge University,  
Pembroke Street,  
Cambridge CB2 3QZ,  
Cambridge, United Kingdom  
email: [pdb1000@cus.cam.ac.uk](mailto:pdb1000@cus.cam.ac.uk)

**Post-doctoral Position**  
**Atomic-scale Materials Physics group**  
**Department of Physics, Technical University of Denmark,**  
**Lyngby**

Applications are invited for a post-doctoral research position in the Atomic-scale Materials Physics group at the Department of Physics, Technical University of Denmark. The research area will be

**Atomic-scale simulations of the mechanical properties of metals and alloys**

The postdoc position is part of a research activity "Nanomechanics of metals and alloys" funded by the Danish Research Agency. The main focus of the research is crystal defects, their interactions, and their influence on the mechanical properties of metals. We are particularly interested in the interactions between dislocations and grain boundaries, nanocrystalline materials, and the structure of dislocation cores and grain boundaries. More information can be found at:

<http://www.fysik.dtu.dk/Nanomechanics> .

A Ph.D. degree in a related theoretical field is required, as is computational experience. The position is for one year with the possibility for a second year. The monthly salary will be approximately DKK 23500 to DKK 25500 (GBP 1800 to GBP 2000) depending upon qualifications.

For further information, please contact Research Professor Karsten W. Jacobsen. Applications including C.V., a list of publications and three references should be sent to Prof. Karsten W. Jacobsen, Department of Physics, DTU, Building 307, DK-2800 Kongens Lyngby, DENMARK. Phone: +45 45 25 31 86, Fax: +45 45 93 23 99, Email: kwj@fysik.dtu.dk

## Five Young Researcher Positions

### COMPLEX ATOM MODELLING NETWORK Cambridge - Eindhoven - Madrid - Stuttgart - Trieste

We expect (subject to completion of contract negotiations) to have openings for 5 Young Researchers to work on an EC funded Network to develop atomistic simulation techniques and to perform precise experiments to validate these techniques. These positions should be available from 1st September 2000.

Those involved in the Network and their areas of work within the Network are:

Dr. M.C. Payne - Cambridge

Development of ab initio linear scaling techniques

E-mail: [mcp1@phy.cam.ac.uk](mailto:mcp1@phy.cam.ac.uk)

Dr. C.F.J. Flipse - Eindhoven

Force and conductance measurements using AFM/STM

E-mail: [C.F.J. Flipse@tue.nl](mailto:C.F.J.Flipse@tue.nl)

Professor F. Flores - Madrid

Development of ab initio transport calculations

E-mail: [fernando@uamcal.fmc.uam.es](mailto:fernando@uamcal.fmc.uam.es)

Dr. P. Gumbsch - Stuttgart

Hybrid quantum mechanical-empirical potential simulations

E-mail: [gumbsch@finix.mpi-stuttgart.mpg.de](mailto:gumbsch@finix.mpi-stuttgart.mpg.de)

Dr. A de Vita - Trieste

Molecular dynamics simulations with on-the-flight fitting of potentials

E-mail: [devita@dimca20.univ.trieste.it](mailto:devita@dimca20.univ.trieste.it)

Applications, including a c.v., should be by e-mail to Dr. M.C. Payne or to the relevant member of the network, from whom further details can be obtained, or in writing to Dr. M.C. Payne, TCM Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, UK.

If you wish to find out more details of the work involved please contact relevant member of the Network.

The EC Rules for Young Researchers are that the Researcher must be:

1. aged 35 years or less at the time of appointment by a participant. An allowance to this age limit may be made for the actual time spent in compulsory military or civil service or child care (a maximum of two years per child for the actual time spent off work);
2. a holder of a doctoral degree;
3. a national of a Member State of the Community or of an Associated State or have resided in the Community for at least five years prior to appointment by a participant in the frame of this contract;

and must not be:

1. a national of the state in which the participant's research appointing team is located and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to appointment.

Details of the those countries which are defined as "Associated States" may be found at:

<http://www.cordis.lu/fp5/src/3rdcountries.htm>

## Post-doctoral Position

### Chemistry Department, University of California, Los Angeles

A postdoctoral position is available in the research group of Professor Emily A. Carter in the Chemistry Department at UCLA. In addition to applications research on materials science problems (e.g., ion diffusion and phase transitions in bulk ceramics, metal-ceramic and ceramic-ceramic interface adhesion, and oxidation and embrittlement of metals), the ideal candidate would be interested in and capable of continuing recent development work on embedding methods (a local CI or MP treatment embedded in periodic DFT - c.f. N. Govind, Y. A. Wang, and E. A. Carter., *J. Chem. Phys.*, 110, 7677 (1999)), kinetic energy density functional theory (c.f. Y. A. Wang, N. Govind, and E. A. Carter, *Phys. Rev. B* **60**, 16350 (1999)), ab initio molecular dynamics (c.f. M. R. Radeke and E. A. Carter, *Ann. Rev. Phys. Chem.*, **48**, 243 (1997)) and/or recently funded collaborative project on bridging length scales from the atomistic to the microstructural. The ideal candidate would be either a physicist or a physical chemist with superior skills in applied mathematics and programming, as well as knowledge/expertise in solid state physics, density functional theory, and/or configuration interaction theory.

For further information about the Carter group, go to:

<http://www.chem.ucla.edu/carter/>

The starting salary is \$30K/yr for the first year (depending on level of experience). Medical, dental, and vision benefits are provided. Interested parties should send a curriculum vitae and arrange to have three letters of recommendation sent to:

Prof. Emily A. Carter,  
Dept. of Chemistry and Biochemistry,  
Box 951569,  
UCLA, Los Angeles, CA 90095-1569  
USA

Inquiries may also be sent to [eac@chem.ucla.edu](mailto:eac@chem.ucla.edu).

**Open position at IRRMA  
Post-Doctoral Position at the EPFL (Lausanne)**

Refer for more details to the web-page:

<http://irrmawww.epfl.ch/ap/post-doc.html>

There is currently a post-doctoral position available for a talented and motivated individual at the Institute for Numerical Research in the Physics of Materials (IRRMA) of the EPFL in Lausanne. The position is for one year and can be extended for a second one. The individual will join a research project based on Disordered Network-Forming Materials. (more on <http://irrmawww.epfl.ch/ap/dn.html>) The purpose of this project is to bring the potential of first-principles simulation to this kind of materials. The focus is on the study of atomic-scale phenomena, both from the structural and dynamical point of view. The research activity proceeds in three directions, covering research areas in the physics and chemistry of vitreous materials, of thin dielectric films on silicon, and of aqueous systems. Previous experience with computational techniques based on density functional theory is highly desirable. The interested candidates should send their (1) curriculum vitae, (2) publication list, (3) one or two reprints representative of previous research, and (4) confidential letters of recommendation to:

Alfredo Pasquarello  
IRRMA-EPFL  
PPH-Ecublens  
CH-1015 Lausanne  
Switzerland  
Tel : +41 21 693 44 16  
Fax : +41 21 693 66 55  
E-mail : [Alfredo.Pasquarello@epfl.ch](mailto:Alfredo.Pasquarello@epfl.ch)

## JOB OPENING IN R & D ORGANIZATION FOR DEVELOPER OF QUANTUM METHODS AT MSI

This Senior Scientist will take a lead position in the development of MSI's density functional theory (DFT) products. As a member of the quantum chemistry team, this individual will develop computational methods to improve the performance the programs, derive and implement methods to allow the computation of new properties, and perform validation projects to demonstrate the utility of the program. Candidates should have a PhD in computational chemistry or physics, experience developing large-scale ab initio programs. A knowledge of Fortran is required; knowledge of C++ and experience with solid-state methods are pluses. Experience required with UNIX, NT, and/or Linux operating systems.

This position will be based at MSI headquarters in San Diego California. Persons interested in this position should send their resume to Dominic King-Smith (dks@msi.com). More information about MSI can be found at

<http://www.msi.com/>

**Postdoctoral Research Fellows**  
**The Computational Modelling Group**  
**The National Microelectronics Research Centre (NMRC)**  
**Cork, Ireland**

The Computational Modelling Group at the National Microelectronics Research Centre (NMRC), Ireland has openings for postdoctoral research fellows in the areas of molecular electronics and quantum electronic transport. Well-qualified candidates will be considered for entry-level research scientist positions, which are permanent posts after an 18 month probationary period.

The NMRC is Ireland's largest research centre and currently employs over 200 people. There are fabrication facilities for silicon and compound semiconductor processing and a new national initiative on nanotechnology is underway at the centre. Details are at

<http://nmrc.ucc.ie>

The Computational Modelling Group is a multi-disciplinary effort which is applying a multi-scale simulation approach to problems in microsystems, nanoelectronics and molecular electronics. The group is participating in the European Union's Future & Emerging Technologies research initiative in the areas of nanotechnology information devices and quantum information processing and communication.

We are seeking highly qualified individuals with an interest in applying electronic structure theory to problems related to molecular charge transport, molecular electronics, and molecular implementations of quantum computing. In particular, applications of endohedral fullerenes to nanoscale electronics and quantum computing are being studied. There is an active collaboration with the Physics Department, University College on electronic structure theory. Through the European supported research projects, researchers will interact directly with groups located throughout the EU.

Interested applicants are encouraged to contact;

Dr. Jim Greer, Group Director - Modelling  
NMRC, Lee Maltings, Prospect Row, Cork, Ireland  
Tel: +353 21 904305,  
Fax: +353 21 270271,  
e-mail:jgreer@nmrc.ucc.ie

or to make a formal application to

Ms. Clodagh Gleeson, Personnel Officer  
NMRC, Lee Maltings, Prospect Row, Cork, Ireland  
Tel: +353-21-904232, Fax: +353-21-904058,  
email: careers@nmrc.ucc.ie

**PhD Studentships**  
**COMPUTATIONAL PHYSICS and MATERIALS MODELLING**  
**JOULE PHYSICS LABORATORY, UNIVERSITY OF SALFORD**

Applications are invited for fully funded Ph.D. Studentships in the areas of Computational Physics and Materials Modelling in the Neutron Scattering and Materials Modelling Group. The group uses a wide range of ab-initio and semi-empirical modelling techniques. Some current projects include ab-initio modelling of the dynamical structure factor in metal hydrides, dynamical properties of ice and structural and magnetic phase transitions in intermettalic hydrides. The group has extensive computational resources including several unix workstations and a 17.2GFlop IBM SP parallel computer.

A variety of funding routes exist including EPSRC quota studentships (UK nationals only) and University Scholarships enhanced by ORS grants for non EU nationals.

For further information please contact:

Dr. Ian Morrison  
Joule physics Laboratory  
University of Salford, UK  
email: i.morrison@salford.ac.uk  
tel: +44 161 2955303

## 8 Abstracts

### On-site Coulomb interaction and exchange splitting in Ni $2p$ photoemission of ferromagnetic nickel

G. van der Laan, S. S. Dhesi and E. Dudzik

*Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK*

#### Abstract

The  $2p$  photoemission of Ni metal displays a weak magnetic circular dichroism (MCD) with a complex structure over an energy range of more than 35 eV. Since a one-particle model clearly fails to explain this experimental result, we propose a Final-State Impurity (FSI) model which assumes that the core-ionized atom can be described as an impurity state in a many-body approach. From this model we obtain the value of the on-site Coulomb interaction  $U$  without having to rely on assumptions concerning the nature of the ground state, which might be either localized or itinerant. The  $\underline{pd}^8$  satellite, which is much more pronounced in the MCD than in the isotropic spectrum, can be used to fix the value of  $U$  to  $\sim 5.15$  eV. We demonstrate that an Anderson impurity model would require different values of  $U$  and transfer integral,  $T$ , in initial and final state. We further present the calculated spin-polarized Ni  $2p$  photoemission. Its  $2p_{1/2}$  structure shows distinct differences with the MCD, which means that the  $2p3d$  Coulomb interaction cannot be neglected with respect to the  $2p$  spin-orbit interaction.

(Accepted for Phys. Rev. B)

Preprints available from: [g.vanderlaan@dl.ac.uk](mailto:g.vanderlaan@dl.ac.uk)

# Interpreting STM-images of the MnCu/Cu(100) surface alloy

D. Wortmann<sup>1</sup>, S. Heinze<sup>1,2</sup>, G. Bihlmayer<sup>1</sup>, and S. Blügel<sup>1</sup>,  
<sup>1</sup> *Institut für Festkörperforschung, Forschungszentrum Jülich,*  
*D-52425 Jülich, Germany*  
<sup>2</sup> *Zentrum für Mikrostrukturforschung, Universität Hamburg,*  
*D-20355 Hamburg, Germany*

## Abstract

$c(2\times 2)$ MnCu/Cu(100) is an ordered two-dimensional surface alloy which exhibits a checkerboard arrangement of Mn and Cu atoms on the Cu(100) surface. Mn buckles outwards by 0.3 Å with respect to Cu and in all previous scanning tunneling microscopy (STM) experiments only one chemical species was imaged which was assumed to be Mn. We analyze the STM results by first-principles calculations based on the density-functional theory and show that Cu rather than Mn is imaged, while indeed Mn is imaged as single Mn impurities at Cu(100). We explain this result in terms of the formation of Mn-states bridging over the Cu atoms. These Mn-states are characteristic for Mn in a  $c(2\times 2)$ MnCu surface alloy. Missing Mn atoms break this bridging bond and the surrounding Cu atoms are imaged as depressions.

(Accepted by Phys. Rev. B )

Copy available from: s.bluegel@fz-juelich.de

Acknowledgement includes: Program Training and Mobility of Researchers 'Interface Magnetism' (Contract: EMRX-CT96-0089) and 'Electronic Structure' (Contract: FMRX-CT98-0178) of the European Union.

# Penetration depth and its doping dependence in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

Z. Szotek<sup>†</sup>, B.L. Gyorffy<sup>‡</sup>, and W.M. Temmerman<sup>†</sup>

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Tyndall Avenue, Bristol, BS8 1TL, United Kingdom*

## Abstract

Using the quasiparticle spectra in the superconducting state, as determined by the eight-band model for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) and a phenomenological interaction constant  $K$ , we have calculated the magnetic penetration depths  $\lambda_a$  and  $\lambda_b$ , respectively along  $a$  and  $b$  axes, as functions of temperature  $T$ , for various levels of oxygen doping. Given that these calculations involve no adjustable parameters the quantitative comparison with the experimental data yields satisfactory agreement. Moreover, the theoretical results reproduce the empirical relationship between  $\lambda(T)$  and doping  $n$ , as well as, the so-called Uemura plot of  $1/\lambda^2(0)$  vs.  $T_c$ . We conclude that the low frequency superconducting electromagnetics of YBCO is governed by a simple BCS-like theory in the context of a realistic description of the normal state electronic structure.

(Phys. Rev. B, accepted, August 1, 2000)

Manuscripts available from: Z.Szotek@dl.ac.uk

# Overlayers, interlayers, and surface alloys of Mn on the Cu(111) surface

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*Institut für Festkörperforschung, Forschungszentrum Jülich,  
D-52425 Jülich, Germany*

## Abstract

The energetics of various surface alloys of manganese on copper (111) are calculated and their stability against clustering and/or interdiffusion is determined by an *ab initio* method. The interplay between stoichiometry, chemical, and magnetic ordering allows for a large variety of ordered alloys; only two are found to be stable against clustering: a 33% alloy and a 50% alloy of antiferromagnetically ordered Mn chains. Thermodynamic considerations indicate that only the 33% alloy will be formed at temperatures typical for epitaxial growth. The results are compared to recent STM experiments.

(Accepted by Phys. Rev. B )

Copy available from: [g.bihlmayer@fz-juelich.de](mailto:g.bihlmayer@fz-juelich.de)

Acknowledgement includes: Program Training and Mobility of Researchers 'Interface Magnetism' (Contract: EMRX-CT96-0089) and 'Electronic Structure' (Contract: FMRX-CT98-0178) of the European Union.

# Fully unconstrained noncollinear magnetism within the projector augmented wave method

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Sensengasse 8, A-1090 Wien, Austria*

## Abstract

Spin-polarized calculations in solids have generally been confined to a global quantization axis to simplify both the theoretical model and its implementation in self-consistent codes. This approximation is justified as many materials exhibit a collinear magnetic order. However, in recent years much interest has been directed towards noncollinear magnetism in which the magnetization density is a continuous vector variable of position. In this paper we develop the all-electron projector augmented wave (PAW) method for noncollinear magnetic structures, based on a generalized local-spin-density theory. The method allows both the atomic and magnetic structures to relax simultaneously and self-consistently. The algorithms have been implemented within a powerful package called VASP (Vienna *ab-initio* simulation package), which has been used successfully for a large variety of different systems such as crystalline and amorphous semiconductors, simple liquids and transition metals. The approach has been used to study small clusters of Fe and Cr, some of these clusters show noncollinear magnetic arrangements.

(submitted to: Phys. Rev. B)

Latex-file available from D. Hobbs at: david.hobbs@univie.ac.at

# Fully unconstrained noncollinear magnetism in triangular Cr and Mn monolayers and over-layers on Cu(111) substrates

D. Hobbs and J. Hafner

*Institut für Materialphysik and Centre for Computational Material Science,  
Sensengasse 8/12, A-1090 Wien, Austria*

## Abstract

A recently developed fully unconstrained approach to noncollinear magnetism has been applied to the investigation of the magnetic ground-state of triangular freestanding Cr and Mn monolayers and over-layers on Cu(111) substrates. Such systems represent a physical realization of a frustrated two-dimensional antiferromagnet. We find that the ground state of the Cr monolayers is noncollinear, it shows  $\sqrt{3} \times \sqrt{3}$  periodicity with  $\pm 120^\circ$  angles between the directions of the magnetic moments on neighbouring sites. Mn monolayers on the other hand have a collinear ground-state with antiferromagnetically coupled rows and  $2 \times 1$  periodicity. The fully unconstrained description allows for a detailed investigation of the spin-densities in the interstitial regions.

(submitted to: J. Phys.:Condens. Matter)

Latex-file available from D. Hobbs at: david.hobbs@univie.ac.at

# Relation between X-ray Magnetic Linear Dichroism and Magnetocrystalline Anisotropy

Gerrit van der Laan

*Daresbury Laboratory, Warrington WA4 4AD, UK*

## Abstract

In itinerant 3d transition metal systems the magnetocrystalline anisotropy energy is directly related to the anisotropic part of the spin-orbit interaction, rather than to the orbital part of the magnetic moment as assumed previously. The spin-orbit anisotropy can be obtained by applying the sum rule for x-ray magnetic linear dichroism (XMLD). This provides an element specific tool to study metallic multilayer systems displaying novel magnetic properties, such as perpendicular magnetic anisotropy.

(Submitted to Lecture Notes, *Magnetism and Synchrotron Radiation*, Mittelwihl 2000, Eds. E. Beaurepaire, *et al.*)

Preprints available from: g.vanderlaan@dl.ac.uk

# Surface stoichiometry and the initial oxidation of NiAl(110)

Alexander Y. Lozovoi, Ali Alavi, and Michael W. Finnis

*Atomistic Simulation Group, School of Mathematics and Physics,*

*The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland, UK*

## Abstract

Selective oxidation of the surface of an ordered alloy requires redistribution of the atomic species in the vicinity of the surface. This process can be understood in terms of the formation and movements of point defects in the compound. On the basis of *ab initio* density-functional calculation we found both the creation of exchange defects near the NiAl surface and segregation of Ni vacancies to the top layer to be extremely favorable in the presence of oxygen. Scenarios for the initial oxidation of NiAl are suggested which demonstrate the appearance of an additional energy barrier on Ni-rich side compared to the Al-rich side. The expulsion of Ni from the oxide layer as it forms is the driving force for its stability.

(To appear in Physical Review Letters)

Manuscripts available from: m.finnis@qub.ac.uk

# Equilibrium and adhesion of Nb/sapphire: the effect of oxygen partial pressure

Iskander G. Batyrev<sup>1,2</sup>, Ali Alavi<sup>1</sup> and Michael W. Finnis<sup>1</sup>

<sup>1</sup>*Atomistic Simulation Group, School of Mathematics and Physics,  
The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland, UK*

<sup>2</sup>*The University of Texas at Austin, Department of Physics,  
Austin, Texas 78712-1081*

## Abstract

We derive a formula, useful for first-principles calculations, which relates the free energy of an oxide/metal interface to the free energies of surfaces and the work of separation of the interface. We distinguish the latter *mechanical* quantity from the *thermodynamic* work of adhesion, and we describe explicitly how both may be calculated. Our formulae for interfacial and surface energies are cast in terms of quantities which can be calculated or looked up in tables, and include as additional parameters the ambient temperature and partial pressure of oxygen  $P_{O_2}$ . From total energy calculations for the Nb(111)/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (0001) interface, free Nb and Al<sub>2</sub>O<sub>3</sub> surfaces, we obtain firstly numerical estimates of the works of separation, which are independent of  $P_{O_2}$ . We then obtain surface energies, interfacial energies and the equilibrium work of adhesion as a function of  $P_{O_2}$ .

(To appear in Physical Review B)

Manuscripts available from: m.finnis@qub.ac.uk

# Point Defects in NiAl alloys under pressure

Alexander Y. Lozovoi<sup>(1)</sup>, Ali Alavi<sup>(1)</sup>, Pavel A. Korzhavyi<sup>(2)</sup>,  
and Michael W. Finnis<sup>(1)</sup>

<sup>(1)</sup> *Atomistic Simulation Group, School of Mathematics and Physics,  
The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom*

<sup>(2)</sup> *Condensed Matter Theory Group, Physics Department, Uppsala University,  
SE-751 21 Uppsala, Sweden*

## Abstract

We investigate the effect of elevated pressures on the point defect thermodynamics in NiAl alloys. A particular motivation for this study is due to the expected elimination of structural vacancies on the Al-rich side at high pressure. We employ the density functional theory to compute point defect energies as a function of pressure, which are in turn used as input to the Wagner-Schottky model. We find that at about 200 kbar a change in the constitutional defect from  $V_{Ni}$  to  $Al_{Ni}$  does take place. The extension of the Wagner-Schottky model by introducing elastic interactions between defects leads to the prediction of a qualitatively new phenomenon in the system, namely the appearance of an isostructural phase transition terminated at a critical point. Similar behaviour is expected in some other ordered off-stoichiometric compounds.

(To appear in Proc. 2nd Int. Alloy Conference (IAC-2))

Manuscripts available from: m.finnis@qub.ac.uk

# A parallel implementation of the FP-LAPW method for distributed-memory machines

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85748 Garching, Germany*

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<sup>3</sup>*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,  
14195 Berlin-Dahlem, Germany*

*\*Present adress: UCLA, Dept. of Math., Box 951555, Los Angeles,  
CA 90095-1555, USA*

## Abstract

The *full-potential linearized augmented-plane wave* (FP-LAPW) method combined with density functional theory (DFT) is the most accurate method for calculating the electronic structure, magnetic, vibrational, and structural properties of bulk crystals, defects, and surfaces. In order to meet the high compute power and memory requirements arising when the FP-LAPW method is applied to complex problems, the sequential FP-LAPW code WIEN 97 has been parallelized for distributed-memory machines, and a first implementation on a Cray T3E has been carried out. The parallel program is designed for use on massively parallel systems with several hundred processors. We report on the main parallelization strategies and present performance measurements giving proof of the good efficiency of the T3E version.

(submitted to: Computing in Science & Engineering)

Contact person: Renate Dohmen (red@ipp.mpg.de)

# Symmetric Versus Nonsymmetric Structure of the Phosphorus Vacancy on InP(110)

Ph. Ebert and K. Urban

*Institut für Festkörperforschung, Forschungszentrum Jülich GmbH,  
52425 Jülich, Germany*

L. Aballe, C. H. Chen, K. Horn, G. Schwarz, J. Neugebauer, and M. Scheffler  
*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,  
14195 Berlin-Dahlem, Germany*

## Abstract

The atomic and electronic structure of positively charged P vacancies on InP(110) surfaces is determined by combining scanning tunneling microscopy, photoelectron spectroscopy, and density-functional theory calculations. The vacancy exhibits a nonsymmetric rebonded atomic configuration with a charge transfer level  $0.75 \pm 0.1$  eV above the valence band maximum. The scanning tunneling microscopy (STM) images show only a time average of two degenerate geometries, due to a thermal flip motion between the mirror configurations. This leads to an apparently symmetric STM image, although the ground state atomic structure is nonsymmetric.

(submitted to: Phys. Rev. Lett.)

Contact person: Günther Schwarz (schwarz@fhi-berlin.mpg.de)

# A Novel STM Imaging Mechanism is Used to Determine the Atomic Structure of the GaAs(001)-(2×4) Surface

V. P. LaBella, D. W. Bullock, Z. Ding, C. Emery, and P. M. Thibado  
*Dept. of Physics, Univ. of Arkansas, Fayetteville, AR 72701, USA*

P. Kratzer and M. Scheffler

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,  
14195 Berlin-Dahlem, Germany*

## Abstract

The research group at the University of Arkansas is interested in the surface physics of fabricating III-V semiconductor structures such as GaAs and InP. We are particularly interested in the fundamental properties, such as template structure, diffusion, nucleation and growth. The techniques used are STM, MBE, RHEED, X-ray diffraction, and Hall effect (see the web-site <http://www.uark.edu/misc/mbestm/>). The theoretical work was done at the Theory Department of the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin, Germany. This group uses density-functional theory calculations mainly for the investigation of the atomic and electronic structure of surfaces, as well as the dynamics of surface processes that constitute the atomistic basis of catalysis and crystal growth. The simulation of STM images forms part of this work as an important tool to study the reconstruction of surfaces (see the web-site <http://www.fhi-berlin.mpg.de/th/ht.html>).

(submitted to: Omicron Newsletter)

Contact person: Vincent P. LaBella ([vlabella@comp.uark.edu](mailto:vlabella@comp.uark.edu))

# Energetics of InAs thin films and islands on the GaAs(001) substrate

L. G. Wang, P. Kratzer, and M. Scheffler

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6,  
14195 Berlin-Dahlem, Germany*

## Abstract

We perform *ab initio* calculations to obtain the formation energy of thin InAs films grown on the GaAs(001) substrate. For the island surface morphology, a hybrid method combining *ab initio* calculations and elasticity theory is employed. Our results show that two-dimensional growth is favored for the first monolayer in a wide range of chemical potentials. Additional deposited material may transform the surface morphology into the three-dimensional island growth mode. The driving force behind this surface morphology change is relieving the elastic energy in the films.

(submitted to: Jpn. J. Appl. Phys.)

Contact person: Peter Kratzer (kratzer@fhi-berlin.mpg.de)

# Doping dependence of the superconducting gap in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

Z. Szotek<sup>†,\*</sup>, B.L. Gyorffy<sup>‡</sup>, and W.M. Temmerman<sup>†</sup>

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<sup>‡</sup> *H H Wills Physics Laboratory, University of Bristol, Tyndall Avenue,  
Bristol, BS8 1TL, United Kingdom*

## Abstract

Using the quasiparticle spectra in the superconducting state, as determined by the eight-band model for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) and a phenomenological interaction constant  $K$ , we have studied the doping dependence of the maximum superconducting gap. Surprisingly our results agree qualitatively with the lower of the two energy scales identified in a recent report by G. Deutscher. [?] Thus, we conclude that this coherence energy range  $\Delta_c$ , measured by Andreev reflection, penetration depth, and Raman experiments, is a BCS-like, weak coupling,  $d$ -wave energy gap. Unfortunately, with regard to the other energy scale  $\Delta_p$  our theory has nothing to contribute. Nevertheless, we suggest that it is not a superconducting feature of the spectra.

(Submitted to Physica C)

Manuscripts available from: Z.Szotek@dl.ac.uk

# Weak-stripe magnetic domain evolution with an in-plane field in epitaxial FePd thin films: Model versus experimental results

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E. Dudzik, H. Dürr, S. S. Dhesi, and G. van der Laan

*Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK*

J. B. Goedkoop

*University of Amsterdam, NL-1018 XE Amsterdam, Netherlands*

## Abstract

The magnetic domain structure in thin ferromagnetic films with perpendicular anisotropy is investigated. The effect of an in-plane magnetic field on the presence of domains and the magnetization profile is analyzed within the framework of a one-dimensional analytical model. The general results are reported in a state diagram as a function of the two relevant dimensionless parameters: the quality factor and the ratio of the film thickness to the exchange length. The experimental results, including hysteresis measurements, magnetic force microscopy, and x-ray resonant magnetic scattering obtained on a generic FePd thin layer, are reported and compared to the model.

(Accepted for J. Appl. Phys.)

Preprints available from: [amarty@cea.fr](mailto:amarty@cea.fr)

# X-ray resonant magnetic scattering from FePd thin films

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*Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK*  
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*DRFMC SP2M, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble, France*  
J. B. Goedkoop  
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## Abstract

Depending on the growth conditions, FePd thin films can display a perpendicular magnetic anisotropy associated with chemical order. In competition with the shape anisotropy, this can lead to striped magnetic domains, with moments perpendicular to the film plane. Under these circumstances, magnetic flux closure should occur. The striped domains were studied with soft x-ray resonant magnetic scattering using circularly polarized light to demonstrate the presence of closure domains. Magnetic depth profiling was performed both at the Fe and Pd L3 edge, by measuring the magnetic diffraction peak intensities versus angle of incidence  $\theta$ .

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# Electron correlation and charge transfer at the Ni/Co interface

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## Abstract

The evolving magnetism and electronic structure at the Ni/Co interface have been studied using x-ray absorption spectroscopy (XAS) and x-ray photoemission spectroscopy (XPS) with circularly polarized x-rays. Deposition of ultrathin Ni films of Co grown on Cu(001) results in an intensity enhancement across the Co  $L_{2,3}$  absorption edge. By comparison, the intensity of the Ni  $L_{2,3}$  edge decreases as a function of Ni film thickness. The relative changes in the Ni and Co XAS intensities are interpreted as an electronic charge transfer from the Co to the Ni. Distinct changes in the Co  $2p$  XAS and XPS line shapes after addition of the Ni overlayer imply a modification of the Co  $3d$  electron correlation due to the charge transfer. The change in the electronic structure is related to the interface magnetism using magnetic circular dichroism sum rule analysis.

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# The relationship between Interlayer Spacing and Magnetic Ordering in Gadolinium

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## Abstract

We report on the application of the Local Spin Density Approximation (LSDA) and the Generalized Gradient Approximation of Perdew-Burke-Ernzerhof (PBE) within the Linear Muffin-Tin Orbital Method in both the Atomic Sphere Approximation (LMTO-ASA) and in the Full Potential (FP-LMTO) method to the description of the magnetic coupling within bulk Gd. Using the LMTO-ASA approach to the band structure problem it is found that, at the experimental lattice parameters, the PBE predicts the experimentally observed ferromagnetic (FM) groundstate whereas the LSDA does not. Moreover the nature of the magnetic coupling between successive layers is found to be dependent on the interlayer separation – in particular a reduction of the interlayer spacing will lead to an increased tendency towards FM coupling between successive layers and, conversely, increase of the interlayer spacing will lead to anti-ferromagnetic (AFM) coupling between layers being energetically favourable. A similar interdependence between the interlayer spacing and the magnetic coupling is also observed from calculations using the FP-LMTO method. These observations are used to analyse the nature of the magnetic coupling of the Gd (0001) surface to the underlying FM bulk.

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Manuscripts available from: W.M.Temmerman@dl.ac.uk

## 9 SCIENTIFIC HIGHLIGHT OF THE MONTH

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### **A new theorem for embedding with application to a new hybrid method for difficult composite systems marrying configurational interaction and density functional calculations**

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There are many situations where one would like to do electronic structure calculations but which are too large for *ab initio* treatment. Usually these contain some special central region which one is interested in, but the coupling to the remainder is too strong for one to neglect it entirely. A common approach has been "embedding" where one solves properly for the inner special part of the system, but with some sophisticated treatment of the boundary to represent more or less accurately the influence of the outer remaining part of the system.

The present article reports on two advances in this field. The first advance is a new theorem to achieve embedding. It replaces the outer region by a non-local separable potential (mathematically rather like a pseudopotential) around the boundary, which has been derived from a Hartree-Fock or Density Functional Theory calculation of the electronic structure in the outer region. The mathematics of the theorem is given in the appendix. Possible applications might include large biological molecules such as chlorophyll where one has an active centre around the Mg atom surrounded by a very large region that for some purposes may be rather inactive. The molecule is too large for a calculation on the whole molecule, but a calculation on the central part is sufficient provided one represents adequately the influence on it of the outer part of the molecule, all in the context of density functional theory or Hartree-Fock.

The theorem was discovered in the course of marrying Density Functional Theory (DFT) calculations in the outer region, with Configurational Interaction (CI) calculations in the central

region. This is the second advance reported here, and really occupies the whole paper, so that the theorem is described in that context. It was only later realised that other important applications of the theorem may lie elsewhere.

Hence the main purpose of this article is to introduce a new method for electronic structure calculations on systems that could not really be treated before. We have in mind a composite system such as a transition metal impurity in silicon or in an oxide host, where one small part has an "open shell" electronic structure at which it is necessary to take some configurations into account beyond the usual DFT approach. We want to be able to calculate the term splitting (in the sense of atomic energy levels) and other forms of excited states. Other examples of such composite systems might be defects with vacancies in a covalent material where the cut off dangling bonds may have some "open shell" character, and in biology a molecule such as haemoglobin containing the open shell Fe atom.

So far the only application (beside some simple tests) has been to one and two Ag atoms in solid  $P_2O_5$ , a material used in dosimetry of ionizing radiation. At present only the ground state has been considered, but it has been shown that two silver atoms have a tendency to coalesce into an  $Ag_2$  molecule in the oxide. The method was developed by the group in St.Petersburg including Vladimir Bulatov and Ilia Tupitsyn with the help of Rex Godby, Mike Payne and others in Cambridge and the use of the CASTEP code for the DFT part of calculations. The open shell part of the calculations has been carried out by the Multi-Configurations Self-Consistent-Field (MCSCF) method using the code from the Swedish group of Prof.B.Roos, which has been well used and tested on atoms and molecules including those of open shell character. Both the DFT and MCSCF calculations are of course fully *ab initio* in the usual sense with Hellmann-Feynman forces on the atomic nuclei.

The problem of course is how to marry DFT and MCSCF calculations because they represent such very different approaches. This is accomplished using two tricks, as we will describe below, the second of which is highly non-trivial and depends on a new theorem which may well have applications in other types of matching calculations. But first a few remarks about the MCSCF calculations are in order since they have not featured much in the Psi-k Newsletter. In an electronic structure calculation on, say, a single Fe atom, one wants to take two types of effects into account involving the mixing of several (or many) determinants in the wave function. The first is the energy splitting between different "terms"  $^5F$  and  $^3P$  etc (in the nomenclature of atomic energy levels) within the same  $3d^74s$  configuration. Even in the lowest Hartree-Fock approximation, the wave function is not a single determinant (as is sometimes alleged) but for an atom is a linear combination of several determinants all from the same  $3d^74s$  configuration, with Clebsh-Gordon coefficients to make the whole an eigenfunction of  $L^2$  and  $S^2$  operators with appropriate  $L(L+1)$  and  $S(S+1)$  eigenvalues. The ideas are extended to molecules and small clusters using  $S^2$  and appropriate spatial symmetry. The second effect to be demonstrated by mixing in more determinants is electron correlations. For an atom this would mean determinants from a higher configuration constructed from a suitable basis set of local orbitals. For a cluster with low symmetry the two effects are mixed together.

In conclusion, therefore, the MCSC method uses an expansion in determinants for the wave function, where each determinant is constructed out of localized orbitals (usually atomic-type

orbitals) chosen to give good convergence for term splittings and correlation, based on experience in quantum chemical calculations. The Achilles heel of the MCSCF method is, of course, that the number of determinants grows exponentially with the size of the system which makes it impossible for solid applications by itself.

We now turn to the two tricks needed to marry the MCSCF and DFT methods. The first trick is illustrated in Fig.1, where space is divided into three regions, with the region I containing the "open shell" part of the system and regions II and III amenable to DFT calculations. In the case of Fe as a substitutional impurity in Si, region I would be the Fe atom, region II the four Si neighbours plus the twelve other bonds that they make to further neighbours, while III is the rest of the Si in the supercell (Fig.2). The MCSCF calculations are carried out in the whole of regions I+II, while the DFT calculations comprise regions II+III. The overlap region II treated by both methods will serve to match the two types of calculation. From DFT calculations of regions II+III an influence of III onto II is extracted which will serve as an embedding potential for MCSCF calculations of regions I+II. Similarly, from MCSCF calculations of the regions I+II the influence of I onto II is extracted to be used as an embedding potential for DFT calculations for regions II+III.

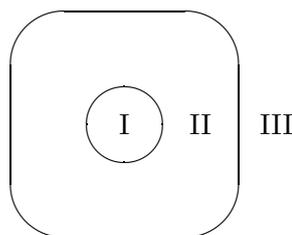


Figure 1: The three regions.

The method is not confined to impurities or defects in a bulk solid. For example regions II and III may be a solid with a surface in the usual "slab" representation, while region I is an adatom on the surface. For haemoglobin region I would be the Fe atom, region II its close neighbourhood, and region III the distant part of the molecule.

We turn now to the second trick, which is the crucial one, with the new theorem and wider application.

It concerns what we do at the outer surface of region II when doing the cluster calculations on I+II, to represent the fact that there is the region III outside the boundary. Let us introduce the issue like this: when people have wanted to do an electronic structure calculation related to something in bulk amorphous Si, they have sometime used a finite cluster and terminated the dangling bonds of the outermost Si atoms with hydrogen atoms. It was found that the covalent bond between an outer Si atom and its H atom is rather similar to that between two Si atoms. Thus from the point of view of the outer Si atom, the H does a fairly good job of replacing the bulk amorphous Si that has been chopped off to make the finite cluster. The new theorem enables us to construct a non-local separable hermitian potential operator  $V'_{sep}$  to do

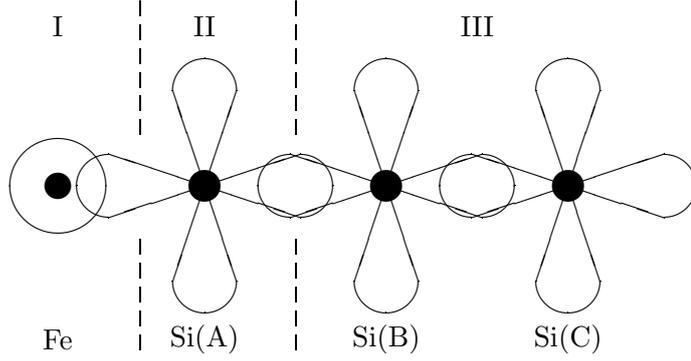


Figure 2: An Fe impurity atom in a Si host crystal.

the job exactly. The  $V'_{sep}$  is a hydrogen-like potential in the sense that it carries one electron, not four, and hence terminates the cluster. But  $V'_{sep}$  is also silicon-like in that its filled "valence" eigenstate is a silicon directed  $sp^3$  hybrid type valence orbital, whose bond to an outer Si atom of the region II is exactly the same as that from a proper Si atom. At the same time the empty "conduction band" states of Si are preserved in  $V'_{sep}$ .

The precise definition of region II for our system when calculating on region I+II is therefore as shown by Fig.3. It includes the inward pointing hybrid and terminating potential  $V'_{sep}$  of Si(B). But in calculating region II+III the Si(B) atom is a full Si pseudopotential (Fig.2). Similarly the Fe atom could be represented by a constructed terminating potential in the LDA calculation on system II+III but in this case it would be easiest and best just to use an Fe DFT potential, at least for a ground state calculation.

The theorem in its simplest form runs like this. Suppose we have the Hamiltonian

$$H_0 = -\frac{1}{2}\nabla^2 + V, \quad (1)$$

where  $V$  is an ordinary potential, and this  $H_0$  has eigenvalues  $\epsilon_n$  and eigenfunctions  $\psi_n$

$$H_0\psi_n = \epsilon_n\psi_n. \quad (2)$$

We can now construct

$$H = H_0 + V_{sep} \quad (3)$$

such that its eigenvalues and eigenstates are as follows

$$\begin{aligned} H\psi'_n &= \epsilon_n\psi'_n, & n > 1 \\ H\phi &= E\phi \end{aligned} \quad (4)$$

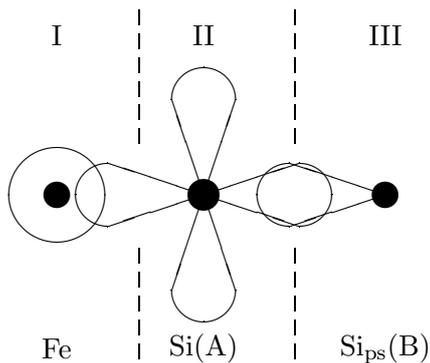


Figure 3: A pseudo-Si directed valence orbital modelling the influence of region III.

where  $E$  and  $\phi$  are given. From (1) and (3), the desired  $V'_{sep}$  is

$$V'_{sep} = V + V_{sep} \quad (5)$$

the lowest eigenstate is the desired  $\phi$  with desired  $E$ , and all the higher eigenvalues  $\epsilon_n (n > 1)$  are preserved. The theorem shows that  $V_{sep}$  has the form

$$V_{sep} = \sum_{i,j=1}^3 |f_i\rangle U_{ij} \langle f_j| \quad (6)$$

where

$$f_1 = \phi, \quad f_2 = \psi_1, \quad \text{and} \quad f_3 = H_0\phi, \quad (7)$$

and where the  $U_{ij}$  involve  $E$ ,  $\epsilon_1$ , and various scalar products of  $f_i$ . The precise form of the  $U_{ij}$  and the proof of the theorem are given in the mathematical appendix.

The use of the theorem in our example is not completely straightforward. The  $\phi$  is our desired  $sp^3$  type hybrid directed valence orbital, pointing towards an outer Si atom of region II. But we do not know a priori what  $\phi$  is, nor its appropriate  $E$ . What we can get from a DFT calculation on pure Si is a set of identical bonding orbitals  $\phi_{bj}$  centered at each bond  $j$  in the crystal. The set of all  $\phi_{bj}$  span the same functional space as the set of Bloch functions of the the valence bands  $\psi_k$  and  $\phi_{bj}$  is constructed as linear combinations of  $\psi_k$ . The  $\phi_{bj}$  can be chosen to be as localized as possible, or to have maximum bond order. The  $\phi_{bj}$  are not mutually orthogonal (unlike the Wannier functions) but one can define matrix elements between them and an energy  $E$  from which the valence band structure can be generated again. The  $\phi_b$  can be thought of as the sum of two hybridised  $sp^3$ -like orbitals on the two atoms, but there is no unique way of splitting up  $\phi_b$  in that way. Therefore the theorem is applied to the pair of atoms and a pair of  $V_{sep}$  are produced which together give  $E$  and  $\phi_b$  exactly. The calculations proceed iteratively

from approximate atomic  $V$ 's in (1) which have been tuned to give some quantity such as the correct lowest excited states of Si or the bottom of the conduction band of bulk Si and this is of course conserved by the operation of the theorem.

As already remarked, the method in its simplest form has been applied to Ag atoms in  $P_2O_5$  including their movement to coalesce into  $Ag_2$  dimers. Both the  $3d^{10}$  and  $3d^9 4s$  configurations had large amplitudes in the ground state and were particularly involved in the dimer formation.

Finally, the group in St.Petersburg WOULD WELCOME COLLABORATORS to apply and develop the method further. Please contact Prof Igor Abarenkov at e-mail: aiv@iva.usr.pu.ru .

### Mathematical appendix

We now define the  $V_{sep}$  and prove the theorem by constructing the required  $H$  of equations (3) and (4). It is convenient to change the notation slightly and to refer to all the eigenvalues and eigenstates of  $H$  by  $\epsilon'$  and  $\psi'$  and we have  $\epsilon'_n = \epsilon_n$  for  $n > 1$ . Thus the  $V_{sep}$  of (6) now has

$$f_1 = \psi'_1, \quad f_2 = \psi_1, \quad \text{and} \quad f_3 = H_0 \psi'_1. \quad (8)$$

We start by considering the unitary transformation  $U$

$$U = I - 2P, \quad (9)$$

where  $P$  is the projector operator

$$\begin{aligned} P &= a |\psi_1 + \psi'_1\rangle \langle \psi_1 + \psi'_1| \\ a &= 1/[2(1 + \langle \psi_1 | \psi'_1 \rangle)] \end{aligned} \quad (10)$$

with the properties

$$P^+ = P, \quad \text{and} \quad P^2 = P, \quad (11)$$

from which the unitary property  $UU^+ = I$  follows readily. Here we employed the fact that by adjusting the phase factors of  $\psi_1$  and/or  $\psi'_1$  the scalar product  $\langle \psi_1 | \psi'_1 \rangle$  can always be made real. We also have

$$(H_0 P)^+ = P H_0 = a |f_1 + f_2\rangle \langle \epsilon_1 f_2 + f_3| \quad (12)$$

We now construct the set of  $\psi'_n$  by the unitary transformation  $U$  operating on the set of  $\psi_n$ :

$$|\psi'_n\rangle = U |\psi_n\rangle. \quad (13)$$

We can now write down the  $H$  that has the required eigenstates and eigenvalues

$$\begin{aligned} H &= \sum_n |\psi'_n\rangle \epsilon'_n \langle \psi'_n| = \sum_n |\psi'_n\rangle \epsilon_n \langle \psi'_n| + |\psi'_1\rangle (\epsilon'_1 - \epsilon_1) \langle \psi'_1| \\ &= U H_0 U^+ + |\psi'_1\rangle (\epsilon'_1 - \epsilon_1) \langle \psi'_1| \end{aligned} \quad (14)$$

where we have written  $\epsilon'_n = \epsilon_n + (\epsilon'_n - \epsilon_n)$  and used the fact that  $\epsilon'_n = \epsilon_n$  except for  $n = 1$ . From (10) and (14) we now have

$$V_{sep} = [UH_0U^+ - H_0] + |\psi'_1\rangle (\epsilon'_1 - \epsilon_1) \langle\psi'_1|, \quad (15)$$

and it remains to simplify the term in square brackets which will turn out to have the required form (6), (8) as the last term of (15) already does. We have from (9), (11)

$$UH_0U^+ - H_0 = -2PH_0 - 2H_0P + 4PH_0P \quad (16)$$

where from (12)  $PH_0$  already has the required form (6), and so does  $H_0P = (PH_0)^+$ . Finally for (16), (15) we need

$$PH_0P = a^2|\psi_1 + \psi'_1\rangle \langle\psi_1 + \psi'_1|H_0|\psi_1 + \psi'_1\rangle \langle\psi_1 + \psi'_1|, \quad (17)$$

where the inner matrix element has the value

$$\langle\psi_1 + \psi'_1|\epsilon_1\psi_1 + H_0\psi'_1\rangle = \langle f_2 + f_1|\epsilon_1f_2 + f_3\rangle, \quad (18)$$

which we denote by  $b$ . Thus

$$PH_0P = a^2b(|f_1\rangle \langle f_1| + |f_1\rangle \langle f_2| + |f_2\rangle \langle f_1| + |f_2\rangle \langle f_2|) \quad (19)$$

and collecting everything from (15) to (19) gives  $V_{sep}$  in the required form (6) with (8), where all the  $U_{ij}$  coefficients (not to be confused with the operator  $U$  in (9)) depend on scalar products of the  $f_i$  which are all calculable.