Ψ_k Newsletter

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

Number 30 December 1998

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Contents

1 Editorial

This Newsletter is rather large and contains a lot of information. In particular, in the **General News** section there is an information on the time and place of the next Psi-k Conference, and Mike Finnis and Jürgen Hafner share with us their thoughts on publishing in European journals. In addition, the Newsletter contains reports on a variety of workshops, and they can be found in the respective sections dedicated to the TMR1 and TMR2 networks, and the ESF programme. All reports contain abstracts of talks presented at those workshops. The section **News from the ESF Programme** contains also a progress report for 1998, and gives all available information on workshops planned for 1999. There we also have some reports on recent collaborative visits. With respect to collaborative visits, we would like to encourage our readers from countries supporting the ESF Programme to submit to us proposals for collaborative visits for 1999.

As usually, in this Newsletter we have a number of job announcements and more abstracts in the standard **Abstracts** section. This time the Newsletter contains also announcements of interesting physics books, published recently by the members of our European Psi-k community.

The scientific highlight is by *A. Ayuela, J.-L. Mozos, R. M. Nieminen, and M.J. Puska* (Helsinki University of Technology) on **"Nanowires: electronic and ionic structures, cohesive and transport properties**.

We would like to encourage our readers to check the content list for more details.

Since, this is the last Newsletter of this calendar year we would like to take this opportunity and wish all our readers **a Merry Christmas and a very Happy New Year**. Also, we would like to thank all of you for contributions to the Newsletters. We hope that next year's Newsletters will be as successful as the ones of the past five years. As always, we count on our readers to contribute any interesting material and to help us to improve the content of the future Newsletters. The first Newsletter of 1999 will be the February issue.

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

http://www.dl.ac.uk/TCSC/HCM/PSIK/main.html

The above contains pointers to home pages of some of the members of our electronic structure community. If you maintain a home page on your activities we will be happy to include a pointer from the *Networks'* home page to your home page.

Please note that the home page of the Psi-k Networks has recently been updated. It contains useful information regarding funding of workshops and collaborative visits within the ESF Programme. Its major new feature is a separate highlight section which contains all highlight articles of the Newsletters published so far.

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

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

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

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

2 General News

2.1 Psi-k2000

Conference on

"Ab initio (from Electronic Structure) Calculations of Complex Processes in Materials"

Schwäbisch Gmünd, 22-26 August, 2000

The good news is that we have decided on the venue and dates for the next Psi-k Conference, the successor of the very successful Schwäbisch Gmünd conference that took place on 17-21 September, 1996.

After reviewing a number of venues in the United Kingdom and Germany, it has been decided that going back to Schwäbisch Gmünd is the preferred option. The conference will take place on 22-26 August, 2000. It will start with registration on Tuesday afternoon, August 22, and finish late afternoon on Saturday, August 26. Unlike the last Schwäbisch Gmünd conference, which was organised by the EU Human Capital and Mobility funded network, its successor will be organised by three networks, namely TMR1, TMR2 and ESF, representing the whole Psi-k community in Europe. As before, it will be open to all and will cover all aspects of the *ab initio* calculations of complex processes in materials. Details concerning the programme, participation, accommodation and funding will be available in due course. It is expected that up to 400 people from all over the world will attend the conference. In order to make this conference as successful as the last conference, please do make a note of it in your calendars.

The conference will be organised by the Daresbury Laboratory node, with Paul Durham as the chairman of the Local Organising Committee.

2.2 Publishing in Europe

Must first-class European research necessarily be published in the US ?

In our last proposals to the EU Commission and to the European Science Foundation for creating the Ψ_k-TMR Networks and the Ψ_k-ESF Research Programme we have been proud enough to claim that in our field Europe has taken the lead over the US and Japan. We think that the development over the last few years demonstrates that such a statement is largely justified. On the other hand we continue to send the best of our work to American Journals such as Physical Review Letters, Physical Review, Journal of Chemical Physics, etc. Only if month-long haggling with the referees of PRL is fruitless, the second attempt is perhaps with Europhysics Letters or the Letter sections of the Journal of Physics or of the new European Journal of Physics. In the meantime priority is often lost.

Should we not also become more selfconscious in the publication of our results (and contribute in the way to the survival of European scientific journals) ? As a member of the Executive Board of the Journal of Physics: Condensed Matter (JPCM) and as a Co-Editor of Europhysics Letters, respectively, we are entitled to decide rapidly on the publication of Letters sent directly to us. Full papers submitted to JPCM via an Executive Board Member are only sent to one further referee and are therefore likely to be processed more quickly. We invite the Ψ_k community to take advantage of this opportunity. Of course we are vitaly interested in maintaining a very high standard - in the interest of our journals as well as in the interest of the community.

Mike Finnis
Executive Board, Journal of Physics: Condensed Matter

Jürgen Hafner
Co-Editor, Europhysics Letters

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Report on Workshops

3.1.1 Report on TB-LMTO Workshop

Workshop on

" The TB-LMTO method "

Mont Sainte Odile, France

October 2-5, 1998

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

The workshop was attended by 67 scientists from 17 different countries (from Europe, Argentinia and Brasil to India, Japan and Australia). The aim of the workshop was to discuss the latest developments in the TB-LMTO method and its advantages, as compared to the usual LMTO method, as well as other band structures schemes. In a lively atmosphere, discussions continued well after the talks. Besides the 14 invited talks, 19 shorter presentations offered the opportunity to focus on more precise points.

O.K. Andersen (Stuttgart) began the meeting by presenting the third generation TB-LMTO method. One of the aim of this method is to overcome the limitations induced by the popular ASA (Atomic Sphere Approximation). In third generation method the wave functions are correct not only within the muffin-tin spheres but also in the interstitial region. One of the advantages of the TB-LMTO method is its usefulness for describing disordered systems, like alloys, with the precision of *ab-initio* methods. I. Turek (Brno) gave a convincing review of the TB-LMTO within the CPA (Coherent Potential Approximation) applied to disordered alloys with surfaces. I. Abrikosov (Uppsala) presented a locally self-consistent Green's function method. This order-N method is particularly interesting for systems with a large number of inequivalent sites.

In its conventional implementations, the LMTO-ASA cannot give forces. For that reason full-potential (FP) approaches have been developed. J. Wills (Los Alamos) presented his elegant implementation of the FP-LMTO method, whereas R. Casali (Trieste) showed another scheme based on smooth Hankel functions developed by M. Methfessel. The main limitation of such FP methods is the huge computational effort which inhibits calculations for large systems. J. Kollar (Budapest) presented a *full-density* method, in between ASA and FP, which combines simplicity and accuracy.

In recent years, one of the main successes of the LMTO schemes has been the description of magnetic systems. O. Eriksson (Uppsala) showed accurate calculations of the magnetic anisotropy of bulk and thin films. Non-collinear magnetism in thin films was also studied within the TB-LMTO method and D. Spisak (Vienna) discussed his application to the well-studied Ni/Cu system. Another spectacular use of the TB-LMTO method was given by J. Kudrnovsky (Prague) on the Interlayer Exchange Coupling (IEC). *Ab-intio* formulations of the IEC between non-collinearly aligned magnetic slabs lead to results in very good agreement with experiments.

M. Alouani (Strasbourg) showed the difficulties but also the possibilities to treat the excited states. H. Ebert (Munich) presented the fully relativistic formalism and its applications to spectroscopy, whereas W.M. Temmerman (Daresbury) gave the last contribution of this meeting by presenting a way to describe the localized and delocalized states within the same formalism, stressing an importance of the self-interaction correction within the local spin density approximation to the density functional theory.

Mathematical and numerical problems are often present. In the TB-LMTO method sparse matrices are numerous. J. Scott (Rutherford) gave an introduction to direct methods for the solutions of large-scale linear systems, emphasizing the progressses made in the development of routines which are now available in libraries. D. Stoeffler (Strasbourg) discussed the interest in the recursion method and various applications.

It is not possible in such a report to present all the richness of the talks and discussions. More informations will be available in a special issue of the Springer series " Lectures Notes in Physics" Without any doubt, there is a great interest for physicists to develop and use fast and efficient methods to determine the electronic structure of complex systems. The LMTO method has provided during this meeting the proof of its vitality.

The "Interface Magnetism" TMR network provided the first impulse for this meeting. The ESF support through the program Ψ_k allowed the participation of a large number of scientists. Particularly important was the presence of a large number of PhD students and post-docs. In that sense the meeting was also successful in the transmission and exchanges between different "generations" of physicists. Finally, the local support of the IPCMS (Institut de Physique et Chimie de Strasbourg) was really appreciated.

Hugues Dreyssé

Programme and abstracts

Friday, October 2 (evening): arrival - lunch 19.30

Saturday, October 3

9.00 - 10.15: *O.K. Andersen (Stuttgart)*
Developing the TB-LMTO formalism (1984 version, 1994 version and its recent developments)

10.15 - 10.45: Break

10.45 - 11.30: *I. Turek (Brno)*
Disordered Alloys and Their Surfaces: Coherent Potential Approach

11.30 - 12.15: *I. Abrikosov (Uppsala)*
Order-N Green's function technique and its application in theory of random alloy

12.30 - 14.00: lunch

14.00 - 14.45: *J. Wills (Los Alamos)*
Full potential and force calculations

14.45 - 15.30: *R. Casali and M. Methfessel (Frankfurt/Oder)*
A FP-LMTO method based on smooth Hankel functions

15.30 - 16.15: break

16.15 - 17.00: *J. Kollar (Budapest)*
From ASA towards full potential

17.00 - 18.00: Selected contributed papers: C1-4

19.00 - 20.30: dinner

20.30 - 23.45: Selected contributed papers C5-16

Sunday, October 4

9.00 - 10.00:	*O. Eriksson (Uppsala)* First principle studies of magneto crystalline anisotropy and spin and orbital moments
10.00 - 10.45:	*J. Kudrnovsky (Prag)* Ab initio theory of the interlayer exchange coupling
10.45 - 11.30:	break
11.30 - 12.30:	*M. Alouani (Strasbourg)* Excited states by means of the linear muffin-tin orbital method
12.45 - 14.00:	lunch
14.15 - 15.00:	*J. Scott (RAL, Daresbury)* Sparse direct methods: an introduction
15.00 - 15.45:	*D. Stoeffler (Strasbourg)* Combining Real Space and Tight Binding Methods for Studying Large Metallic Systems
15.45 - 16.30:	break
16.30 - 17.15:	*D. Spisak and J. Hafner (Wien)* Atomic and magnetic structure of nickel films on copper
17.15 - 18.00:	Selected contributed papers C17-19
19.00	banquet

Monday, October 5

9.00 - 10.00:	*H. Ebert(Munich)* Fully relativistic band structures calculations for magnetic solids: formalism and applications
10.00 - 10.45:	*W. Temmerman (Daresbury)* An Unified Band Structure Description of Localized and Delocalized States
10.45 - 11.30:	break
11.30 - 12.30:	*General discussion and concluding remarks*
12.45 - 14.00:	lunch
14.00:	departure to airport

List of contributed papers follows.

C1. *Tanusri Saha-Dasgupta (Stuttgart)*
Tight-binding Modelling using third-generation LMTO method

C2. *Catia Arcangeli (Stuttgart)*
Removing the need of Empty Spheres in the new LMTO-ASA method

C3. *Rashmi Tank (Stuttgart)*
Full charge density expansion and improved total energies in LMTO-ASA calculations

C4. *Nguyen-Manh (Oxford)*
Structural Stability of the Ternary AuCo$_2$(1-u)Sn$_4$ and AuNi$_2$Sn$_4$ Phases via TB-LMTO method

C5. *G. P. Das (Mumbai)*
Phase stability of binary intermetallics : a first-principles tight-binding approach

C6. *N. Kulikov (Troisk)*
B2 transition metals aluminides studied by KKR-CPA and TB-LMTO

C7. *E. Holmstrvm (Uppsala)*
Magnetic Interlayer Coupling in Fe/Pd Multilayers

C8. *J. Izquierdo (Valladolid)*
Electronic and magnetic structure of thin Cr films on Co substrate

C9. *Indra Dasgupta (Stuttgart)*
TB-LMTO: Applications to High Temperature Superconductors

C10. *A. Vega (Valladolid)*
Optical properties of substoichiometric titanium carbides

C11. *A. Vernes (Munich)*
Topological analysis of electronic density in solids

C12. *Z. Szotek (Daresbury)*
TB-LMTO: Applications to electronic properties in the superconducting state

C13. *Biplab Sanyal (Calcutta)*
Study of magnetism of inhomogeneous overlayers

C14. *A. Niklasson (Uppsala)*
Spin-density waves in thin Chromium films

C15. *T. Fujiwara (Tokio)*
TB-LMTO - LDA+U calculations for Spin and Orbital Ordering Nd$_{1-x}$Sr$_x$MnO$_3$

C16. *A. Lichtenstein (KFA-Julich)*
Electronic correlations and magnetism of transition metals

C17. *M. Michalewicz (Melbourne)*
Equation-of-motion O(N) electronic structure studies of large systems (N 10^7)

C18. *A. Niklasson (Uppsala)*
Interface mixing energy; a measure of interface stability

C19. *S. Ostanine (Strasbourg)*
Optical Γ-phonon in hcp Zr: FP-LMTO based approach for pressure and temperature dependencies

Developing the TB-LMTO formalism

O.K. Andersen, T. Saha-Dasgupta, C. Arcangeli, R.W. Tank, G. Krier, O. Jepsen, and I. Dasgupta

MPI-FKF, Postfach 80 06 65, D-70506 Stuttgart, Germany

1. Introduction

2. LMTOs of the seventies

3. LMTOs of the eighties

4. LMTOs of the nineties, and beyond.
    A. Screened Spherical Waves
    B. Structure Matrix
    C. Kinked Partial Waves
    D. Low-energy, few orbital TB-Hamiltonians
    E. LMTOs, Hamitonian and Overlap matrices
    F. NMTOs
    G. Green functions
    H. Largely overlapping potential spheres
    I. Charge density and total energy.

5. Conclusion

Ab initio study of disordered alloys and their surfaces: Coherent potential approximation

Ilja Turek

Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Zizkova 22, CZ-61662 Brno, Czech Republic

Josef Kudrnovský

Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18040 Prague, Czech Republic

Václav Drchal

Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18040 Prague, Czech Republic

1. Introduction

2. Green functions in the atomic sphere approximation

3. Coherent potential approximation
   - 3.1. Site-diagonal quantities
   - 3.2. Non-site-diagonal quantities
   - 3.3. Transformation properties of LMTO-CPA
   - 3.4. Solution of CPA selfconsistency

4. Surfaces and interfaces

5. Charge selfconsistency for random alloys

6. Disordered local moment state
   - 6.1. Paramagnetic state of ferromagnetic metals
   - 6.2. Alloys with strong chemical and magnetic disorder
7. Bulk and surface magnetism of random transition-metal alloys

Lpcally Self-Consistent Green's Function Method and Its Application in Theory of Random Alloys

Igor A. Abrikosov,

Pavel A. Korzhavyi, Börje Johansson

Condensed Matter Theory Group, Physics Department Uppsala University, S-75121 Uppsala, Sweden

1. Introduction $O(N^3)$ vs $O(N)$

2. Locally self-consistent Green's function method
   - 2.1. Assumptions and definitions
   - 2.2. Concept of local self-consistency and effective medium
   - 2.3. Computational algorithm
   - 2.4. Multipole corrections to the ASA
   - 2.5. Taking advantages of tight-binding LMTO represantation
   - 2.6. Electronic properties of surface alloys: tje LSGF method
   - 2.7. Electronic properties of alloys with local lattice relaxations

3. Summary: some applications of the LSGF method

Full potential and force calculations

J.M. Wills

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

1. Introduction

2. Theory
   2.1 full potential implementation
   2.2 atomic relaxation and calculation of forces

3. Applications
   3.1 atomic relaxation for perfect crystals
   3.2 defects and diffusion
   3.3 phonons

4. Conclusion

A full-potential LMTO method based on smooth Hankel functions

M. Methfessel

Institute for Semiconductor Physics, Walter-Korsing-Strasse 2, D 15230 - Frankfurt (Oder), Germany

R. Casali

Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional del Nordeste, Av. Libertad 5600, 3400 Corrientes - ARGENTINA

1. Introduction

2. Smooth Hankel functions
   a. Basic properties
   b. Using the functions to reduce the basis size
   c. Using the functions to reduce the numerical effort

3. Reformulation of the augmentation step
   a. Splitting quantities into smooth and local terms
   b. Hamiltonian and overlap matrix
   c. Charge density and potential
   d. Assembling the output density and forces

4. Sample calculations

From ASA towards Full Potential

Janos Kollar

Research Inst. for Solid St. Physics and Optics, H-1525 Budapest, POB. 49, Hungary

Levente Vitos

Condensed Matter Theory Group, Physics Dept.,Uppsala University, S-751 21 Uppsala, Sweden

Hans L. Skriver

Center for Atomic scale Materials Physics and, Physics Dept., Technical University of Denmark, DK-2800 Lyngby , Denmark

1. Introduction
2. Energy functional
    2.1. Kinetic and Exchange-correlation energy
    2.2. Coulomb energy
3. Construction of the Charge Density
4. Shape function
5. Applications
6. Conclusions

First principles theory of magneto crystalline anisotropy

O. Eriksson

Department of Physics, Uppsala University, Box 530 Uppsala, Sweden

1. Background
2. Solving technical problems, e.g. convergence of k-space integration
3. Examples from the 3d transition metals
4. The strained state of Fe , Co and Ni
5. Overlayers of Ni on Cu
    - MOKE

Ab initio theory of the interlayer exchange coupling

J. Kudrnovský [a,b], V. Drchal [a,b], I. Turek [c],P. Bruno [d], P.H. Dederichs [e], and P. Weinberger [b]

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Excited states by means of the linear muffin-tin orbital method

M. Alouani

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J.M. Wills

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

1. Introduction

2. Theory
    - 2.1 Density functional theory
    - 2.1.1 Kohn Sham equations and the local density approximation
    - 2.1.2 Choice of the basis set
    - 2.1.3 Excited states
    - 2.2 Quasi-particles
    - 2.2.1 The GW-approximation
    - 2.2.2 Excited states and the dielectric function
    - 2.3 The interband transitions by means of the linear muffin-tin orbital method
    - 2.3.1 The spherical potential formulation
    - 2.3.2 The full potential formulation
3. Applications
    - 3.1 Optical properties
    - 3.2 X-ray absorption and magnetic dichroism
    - 3.3 Magneto-optical Kerr effect

4. Conclusion

Sparse direct methods: an introduction

J. Scott

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1. Introduction
2. The general approach
3. Frontal methods
    - 3.1 The multiple front approach
4. Multifrontal methods
5. A comparsion of codes
6. Availability of the codes
7. References

Combining Real Space and Tight Binding Methods for Studying Large Metallic Systems: Magnetically Frustrated Multilayers

Daniel Stoeffler and Clara Cornea

IPCMS-GEMME, 23 rue du Loess, BP-20CR, F-67037 Strasbourg Cedex, France

1. Introduction

2. Tight Binding Parametrization and Recursion Technique
    - 2.1. The Recursion Technique
    - 2.2. Tight Binding Hamiltonian
    - 2.3. Clusters for the Recursion Method
    - 2.4. A practical illustration: the Fe/Cr multilayers

3. Real Space Cell
    - 3.1. Periodic versus Real Space Cells for studying bulk magnetic wall in Cr
    - 3.2. A complete study of the magnetic behaviour of Fe overlayers on Cr substrates
4. Non Collinear Magnetism
    - 4.1. Continuous Fraction Expansion and Non Collinear Magnetism
    - 4.2. Angular Dependance of the Interlayer Magnetic Couplings in Fe/Cr Multilayers
    - 4.3. Step Induced Non Collinear Magnetism

Atomic and magnetic structure of nickel films on copper

D. Spisak and J. Hafner

Institut fuer Theoretische Physik, TU Wien, Wiedner Hauptstrasse 8-10, Austria

1. Introduction

2. TB-LMTO and real-space recursion approach
    - 2.A Magnetocrystalline anisotropy
    - 2.B Exchange coupling constants

    - 3. Ni/(001)Cu films
    - 3.A Atomic structure
    - 3.B Magnetic structure
4. Concusion

Fully relativistic band structure calculations for magnetic solids – Formalism and Application

H. Ebert

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Theresienstr. 37-41, D-80333 München, Germany

1. Introduction
2. Formalism

2.1. Relativistic density functional theory
   - spin density functional theory
   - current density functional theory
   - orbital polarization scheme
   - Breit interaction

2.2. Multiple scattering formalism
   - solution of the single site Dirac equation
   - full potential formulation
   - multiple scattering and Green's function
   - solution of the multiple scattering equations
   - CPA

3. Applications

3.1. Hyperfine interaction

3.2. Magneto-crystalline anisotropy

3.3. Transport properties

3.4. Spectroscopy
   - XAS
   - MEXAFS
   - VB–XPS
   - AES
   - MOKE

An Unified Band Structure Description of Localized and Delocalized States

W.M. Temmerman

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1. Introduction
2. SIC-LSDA Formalism
   a. Non-relativistic
   b. Relativistic
3. Implementation
   a. Steepest Descent Method
   b. Unified Hamiltonian Method
4. Application to Rare Earths and Compounds
5. Application to Strongly Correlated 3d Transition Metal Oxides
6. Conclusions

Tight-Binding Modelling using third-generation LMTO method

Tanusri Saha-Dasgupta

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We show how the improved (third-generation) LMTO method can be employed to obtain tight-binding Hamiltonians. This will be demonstrated by deriving various LMTO sets for the high T_c superconductor and for diamond-structured silicon.

The weak energy dependence and short range of the screened and renormalised KKR matrix will be exploited by using it to generate few orbital, low energy and possibly orthogonal and short-ranged Hamiltonians for a generic high T_c superconductor, while a generalised ASA method will be employed to derive first-principles sp^3 and sp^3d^5 TB Hamiltonians for the valence and lowest conduction bands of silicon.

Removing the need of empty spheres in the new LMTO-ASA method

C. Arcangeli

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By applying the new LMTO method in the test case of diamond-structured Si, we will show that accurate band structure calculations can be performed by using *atom-centred , large overlapping* spheres, without resorting to the introduction of empty-spheres. This is possible because the new LMTO basis set is now complete to first order in energy everywhere in space. Therefore, as for KKR, the energy errors introduced by the use of overlapping muffin-tin wells are only of second order in the potential overlap. We will show that the new atomic-spheres potential can be constructed by a least-squares fit to the full potential in the region accessible to the valence electrons. With the inclusion of correction terms for the overlap error the band structure may be accurately described even at extremely large overlaps.

Full-charge-density expansion for LMTO-ASA calculations

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We show how it is possible in the new LMTO formalism to expand the full, non spherical, charge density using localised screened spherical waves. This is an efficient, real space, scheme which uses a minimal number of expansion functions. Once done, both the solution of Poisson's equation and evaluation of integrals become exact. In this way we can make a more accurate evaluation of the electrostatic contribution to the total energy in a LMTO-ASA calculation. A similar expansion can be made for the exchange correlation energy, and the resulting total energy should be sensitive to non symmetry preserving structural changes in the system.

Furthermore, such a full-charge-density scheme is required for any ASA calculation where the atomic spheres are not space filling.

Structural stability of the ternany $AuCo_{2(1-u)}Sn_4$ and $AuNi_2Sn_4$ phases via TB-LMTO method

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The relative structural stability of the recently discovered ternary phases $AuCo_{2(1-u)}Sn_4$ ($0.167 \leq u \leq 0.180$) and $AuNi_2Sn_4$, the crystal structures of which belong to the NiAs family, are investigated using the TB-LMTO method. It is found that the stability of $AuCo_{2(1-u)}Sn_4$ is governed by strong d-sp bonding occurring in the low symmetric (monoclinic) Ni_3Sn_4-type structure, whereas $AuNi_2Sn_4$ is stabilised essentially by nearly free electron sp bonding in the rhombohedral Fe_3S_4-s-type (mineral smythite) structure. A systematic analysis of the relative total energy across the 3d transition metal (T) row for the ternary AuT_2Sn_4 series shows that the Fe_3S_4-s-type structure tends to be stable when the valence electron number (N) per T atom is < 3.0 or ≥ 9.0, whereas the Ni_3Sn_4-type structure is more stable for $3.0 \leq N < 9.0$. Our calculations are in agreement with the fact that vacancies have to be introduced in $AuCo_{2(1-u)}Sn_4$ in order to stabilise this phase. The spin-polarised electronic structure calculations are in excellent agreement with magnetic susceptibility measurements for both phases.

Results of our TB-LMTO predictions have been verified by fully relaxed *ab initio* supercell calculations in order to explore explicitely the effect of vacancies on the relative stability of $AuCo_{2(1-u)}Sn_4$. It is confirmed that the introduction of vacancies on the Co-sublattice is essential for the occurence of ternary $AuCo_{2(1-u)}Sn_4$ phase with the observed Ni_3Sn_4 structure type.

Onset of magnetism in B2 transition metals aluminides

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We have shown that the onset of magnetism in the Ni, Co and Fe aluminides is closely related to the defect structure of these compounds. The calculations were performed using the KKR-CPA method for the disordered case and the TB-LMTO method for the intermetallic compounds. We studied in particular the onset of magnetism in Fe-Al and Co-Al systems as a function of the point defect structure. We found the appearence of large local magnetic moments associated with the transition metal antisite defect in FeAl and CoAl compounds, in agreement with the experimental findings. Moreover, we found that any vacancies on both sublattices enhance the magnetic moments via reducing the charge transfer to TM atom. Disordered Fe-Al alloys are ferromagnetically ordered, whereas Co-Al becomes magnetic only for Co concentration exceeds equiatonic composition.

Phase stability of binary intermetallics: A first-principles tight-binding approach

G.P. Das

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The linkage between the quantum and the statistical mechanics leading to the first-principles configurational thermodynamics of alloys comes via the configurational energy expression which is expanded in terms of effective pair/multisite (cluster) interactions (EPI). These EPIs have been calculated from first-principles using the TB-LMTO method in conjunction with (a) Connolly-Williams inversion method and (b) augmented space recursion - orbital peeling technique.

We have determined the local density electronic structure and the zero temperature phase stability of the various fcc/bcc based ground state ordered superstructures of $\mathrm{Li}_{1-x}\mathrm{Al}_x$ and $\mathrm{Ni}_{1-x}\mathrm{Mo}_x$ alloys spanning the entire concentration range. Following the 'transferability prescription' of Andersen, we have estimated the potential parameters of the constituent atoms as embedded in the alloy, and compared these with the corresponding charge self-consistent paramters. Our calculated EPIs have been deployed onto some free energy models viz. the 'static concentration wave' model and the 'cluster variation method', in order to determine the ordering and the clustering instabilities present in these alloy systems, as well as the evolutionary path of the order-disorder transformation.

Magnetic Interlayer Coupling in Fe/Pd Multilayers

E. Holmström, A. Niklasson, L. Nordström, I. Abrikosov and B. Johansson

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Magnetic properties of Fe/Pd (100) multilayers have been calculated using a first principles TB-LMTO Green's function method. We investigate how the magnetic interlayer coupling is changed when the magnetic moment of the Fe layers is suppressed. A complex non-RKKY like behaviour of the interlayer coupling as function of Fe magnetic moment was found, indicating the influence of magnetic enhancement effects in Pd. An oscillatory behaviour of the induced

Pd moment as function of Pd spacer thickness is found and explained in terms of quantum confinement.

Electronic and Magnetic structure of thin Cr films on Co substrate

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Kohlhepp *et al* have studied the growth and the magnetic profiles for thin Cr films on Co substrate. More recently Boukari *et al* have reported on the influence of Cr deposition on the magnetic properties of epitaxial Co films grown on Pd(111)

In the present communication we report recent TB-LMTO calculations of a Cr monolayer on fcc Co(100), studing the influence of the interplanar distance in the magnetic properties of the system. In plane ferromagnetic as well as antiferromagnetic configurations have been explored.

TB-LMTO: Application to High T_c superconductors.

Indra Dasgupta

Max-Planck-Institut FKF, D-70569 Stuttgart, Germany

The electronic structure of High T_c cuprates and ladder compounds is discussed in terms of a few orbital tight-binding Hamiltonian obtained from all orbital LMTO Hamiltonian by integrating out high-energy degrees of freedom using a downfolding technique.

We show the resulting chemical Hamiltonian for the High T_c cuprates contains the relevant degrees of freedom necessary to describe the differences between them. In particular, we discuss the influence of apical oxygen and the geometry of the CuO planes on the stationary points of the band structure which gives rise to Van Hove singularities (VHS) in the densities of states close to the Fermi-level, relevant for the Van-Hove Scenario for the cuprates.

We will present a tight-binding model for the ladder compound $SrCu_2O_3$ and discuss the role of pressure on the inter- and intra-ladder hoppings.

Optical conductivity in sub-stoichiometric titanium carbides

J. Izquierdo, A. Vega, S. Bouarab

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Universidad de Valladolid, E-47011 Valladolid, Spain

M. A. Khan

Institut de Physique et Chimie des Matériaux de Strasbourg,
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A theoretical study of the optical absorption of perfectly ordered titanium carbides TiC_x is reported for different carbon concentrations (x=1, 0.75, 0.50, 0.25). The optical conductivity is calculated within the framework of the linear muffin tin orbital (LMTO) method in the atomic sphere approximation (ASA). The effect of carbon vacancies on the optical conductivity is discussed and the origin of the different absorption peaks is traced back to particular interband transitions.

Topological analysis of electronic density in solids

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The theory of the topological analysis of electronic density for atoms in molecules (AIM) developed by Bader has been extended for atoms in solids to study their ionic character. The underlying electronic structures we had calculated using the tight binding linear-muffin-tin-orbital (TB-LMTO) band structure method within the density functional theory (DFT).

All the investigated compounds had either NiAs– or CdI_2–like hexagonal structure and MX or MX_2 chemical formula (M=Ti, V, Cr; X=S, Se, Te). To get a better understanding of the charge transfer, we had calculated for each compound the volume of the polyedron around the atoms and the included amount of charge. It turned out that in all the investigated compounds the bonds are of M–X–type (no M–M bonds were observed) and the ionicity is direct proportional to the splitting between the p– and d–bands.

TB-LMTO: Applications to electronic properties in the superconducting state

Z. Szotek(a), **B. L. Gyorffy**(b), **W. M. Temmerman**(a), **O. K. Andersen**(c), **and O. Jepsen**(c) (a) *Daresbury Laboratory, Warrington, WA4 4AD, UK*

(b) *H H Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, UK*

(c) *Max-Planck-Institut für Festkörperforschung, Postfach 800665, D-70506 Stuttgart, Germany*

We present a semiphenomenological approach for calculating the quasiparticle spectra of High Temperature Superconductors (HTSC's). It is based on a particularly efficient parametrization of the effective electron-electron interaction afforded by the Density Functional Theory for superconductors and a Tight-Binding-Linearized-Muffin-Tin-Orbital scheme for solving the corresponding Kohn-Sham-Bogoliubov-de Gennes equations. We present our results for the gap function on the Fermi surface and compare them with those deduced from photoemission experiments on single crystals of $YBa_2Cu_3O_7$. We also show our predictions for the temperature dependence of the specific heat with measurements. We investigate the doping dependence of the superconducting transition temperature, T_c, and discuss preliminary results for penetration depth. We present new evidence that the Van Hove-like scenario is an essential feature of superconductivity in these materials.

Study of magnetism of inhomogeneous overlayers

Biplab Sanyal and Abhijit Mookerjee

S.N.Bose National Center for Basic Sciences, Calcutta, INDIA

Study of surface magnetism has become one of the major fields of research from the point of view of basic physics and immense technological importance. Moreover, roughness developed during deposition plays an important role in dictating magnetic properties. We here study magnetism of transition metal overlayers on noble metal substrates and the effect of surface roughness, short range ordering and interdiffusion on magnetic properties. We use the methodology of Augmented Space Recursion coupled with Tight-Binding Linearized Muffin Tin Orbital method for this investigation. We show that Fe deposited on Cu(001), Au(001) and Ag(001) as rough monolayer has interesting variations in magnetic moments.

Spin density waves in thin chromium films

A.M.N. Niklasson, Lars Nordström and B. Johansson

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H.L. Skriver

Center for Atomic-scale Materials Physics and Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark

The magnetic structure of thin chromium bcc(001) films (about 50 monolayers) is investigated by means of a first principles TB-LMTO surface Green's function technique. Incommensurate spin density waves are found with a periodicity in good agreement with experiment. The influence of the boundary conditions is studied by the embedding of the chromium films in different surroundings (Fe, Cu, Mo and vacuum). Especially the behaviour of the spin density wave when the magnetic interface alignement is altered is analysed.

Spin and Orbital Ordering of $Nd_{1-x}Sr_xMnO_3$ from LSDA+U calculations

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and

Michael Korotin

Institute of Metal Physics, Russian Academy of Sciences, 620219 Ekaterinburg GSP-170, Russia

The electronic structures of $Nd_{1-x}Sr_xMnO_3$ with $x = 1/2$ (high and low temperature phases) and $x = 9/16$ were studied by using the rotation-invariant LSDA+U formalism

in framework of the LMTO-ASA method. The experimental magnetic structure is calculated to be the energetically lowest one among the different possible spin configurations for every compound under consideration. The orbital ordering is clearly demonstrated by the partial Mn 3d-densities of states projected into a natural local basis for every MnO_6 octahedron.

The mechanism of antiferromagnetic and ferromagnetic couplings in these materials is discussed.

Antiferromagnetic interlayer coupling at $x = 9/16$ is attributed to the crystal structure with an anisotropic shorter interlayer distance.

Electronic correlations and Magnetism of Transition Metals

A. I. Lichtenstein and M. I. Katsnelson

Forschungszentrum Jülich, 52425 Jülich, Germany

We discuss a possibility to include correlation effects in the electronic structure of magnetic crystals. A novel Dynamical Mean Field Theory (DMFT) which takes into account a frequency dependence of the self energy have been combine with the LMTO-TB scheme. The fluctuation exchange (FLEX) approximation and Quantum Monte-Carlo (QMC) method are generalized to the spin-polarized multi-band case. As an example, we calculate the electronic quasiparticle spectrum of ferromagnetic iron using LMTO-TB method in the DMFT-FLEX and DMFT-QMC approximations. It is shown that the Fermi liquid description of the bands near the Fermi level is reasonable, while the quasiparticle states beyond approximately 1 eV range are strongly damped, in agreement with photoemission data.

Equation-of-motion $O(N)$ electronic structure studies of large systems ($N \sim 10^7$)

Marek T. Michalewicz

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An extremely fast implementation of the equation-of-motion method for diagonalisation of a Tight Binding Hamiltonian is presented. The method is solved in real space and hence can be applied to non-periodic, disordered nanocrystalline samples, metals, transition metal oxides and other systems with arbitrary defects. It scales linearly, *O(N)*, runs with a speed of up to 43 GFLOPS/s on NEC SX-4 vector-parallel supercomputer with 32 processors and computes electronic densities of states for multi-million atom samples in mere minutes.

The largest computational test performed was for the TiO_2 sample consisting of 7,623,000 atoms ($48nm \times 50nm \times 32nm$ nanocrystallite) and took 41 minutes on a 16 CPU machine. Mathematically, solving this was equivalent to obtaining a spectrum (electronic density of states DOS) of an $n \times n$ Hermitian operator (Hamiltonian) where $n = 38,115,000$. We discuss practical implications of being able to perform electronic structure computations of this great speed and scale.

Interface mixing energy; a measure of interface stability.

A.M.N. Niklasson, I.A. Abrikosov and B. Johansson

Condensed Matter Theory Group, Physics Department Uppsala University, S-75121 Uppsala, Sweden

As a measure of the thermodynamic stability of metallic interfaces an interface mixing energy is defined and calculated by means of a first principles TB-LMTO Green's function technique for different interfaces of Au/Ag and Cu/Ni. We show that the interface mixing energy is a thickness and directional dependent quantity and the results of our calculations are analyzed in terms of an Ising model. The ratio between the interface and bulk mixing energy is shown to be a valuable quantity which makes it possible to use available bulk data to estimate interface stabilities.

Optical Γ-phonon in hcp Zr: FP-LMTO based approach for pressure and temperature dependencies

S. Ostanin, E. Salamatov, and V.Trubitsin

IPCMS - GEMME, Strasbourg, France

Physico-Technical Institute, RAS, Izhevsk, Russia

The effective potential for $E_{2g}-$ phonon at $\vec{k}$=0 of hcp Zr is calculated for different pressures by the FP-LMTO based frozen-phonon method. The temprerature and pressure dependence

of the phonon frequency ω is studied within the framework of a modified pseudo-harmonic approximation.

The obtained room-temperature results are in good agreement with experimental ones. A change in the behavior of $\omega(P)$ with temperature may be attributed to peculiarities of the phase diagram of Zr.

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 TMR-LAPW Workshop

TMR-Network on 'Electronic Structure calculations of materials properties and processes for industry and basic science'

Jülich, November 6th –7th, 1998

Organised by: **Stefan Blügel** (s.bluegel@fz-juelich.de)

The working group of the FLAPW node of the TMR-network "Electronic Structure calculations of materials properties and processes for industry and basic science" met at the Forschungszentrum Jülich at Nov 6th –7th, 1998, for a 2 days mini-workshop in order to exchange information on the recent progress of the individual members, to investigate and evaluate new approaches to further develop the FLAPW method, and to discuss and coordinate our future node activity.

At first we had a few talks on the realization and capabilities of the existing FLAPW-codes followed by a discussion of coordinated action on improving our codes. In second set of talks we focussed on new algorithmic developments either making the FLAPW method more efficient or branching into new fields and areas. Alternatives of present solutions had been discussed. A third set of talks focussed on applications.

The workshop was attended by about 22 participants. The program of the workshop and the abstracts of all talks are attached. All talks were well received and the discussion took place in a relaxed atmosphere. In total the workshop was rather intense and stimulating and we believe that we are on a good course.

(Stefan Blügel)

PARTICIPANTS:

R. Abt	IFF, Forschungszentrum Jülich, Germany
C. Ambrosch-Draxl	Institut für Theoretische Physik, Karl-Franzens-Universität Graz, Austria
G. Bihlmayer	IFF, Forschungszentrum Jülich, Germany
P. Blaha	Institut für Technische Elektrochemie, TU-Wien, Austria
S. Blügel	IFF, Forschungszentrum Jülich, Germany
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R. Kouba	Institut für Theoretische Physik, Karl-Franzens-Universität Graz, Austria
E. Krasovskii	Institut für Theoretische Physik, Universität Kiel, Germany
P. Kurz	IFF, Forschungszentrum Jülich, Germany
X. Nie	IFF, Forschungszentrum Jülich, Germany
L. Nordström	Physics Department, Uppsala University, Sweden
R. Pentcheva	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
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K. Schwarz	Institut für Technische Elektrochemie, TU-Wien, Austria
E. Sjöstedt	Physics Department, Uppsala University, Sweden
F. Starrost	Institut für Theoretische Physik, Universität Kiel, Germany
T. Thonhauser	Institut für Theoretische Physik, Karl-Franzens-Universität Graz, Austria
X.-G. Wang	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
W. Wolf	Molecular Simulations (MSI), Paris, France

PROGRAM:

Friday, November 6th, 1998

Morning session:

9:00	9:30	**Opening**	S. Blügel	Jülich
9:30	10:30	*Overview of WIEN97 LAPW-code*	K. Schwarz	Wien
10:30	11:15	*Overview of Film/Bulk FLAPW-7-code*	G. Bihlmayer	Jülich
11:15	12:00	*Electronic Excitation Spectra from Non-Local Screened Exchange and Model-GW: Implementations in the Bulk FLAPW Code and Applications*	W. Wolf	Paris
12:00	14:00	**Lunch**		

Afternoon session:

14:00	14:45	*Improving the Efficiency of FP-LAPW Calculations*	M. Petersen	Berlin
14:45	15:45	Round Table discussion: Networking		
15.45	16:00	**coffee break**		
16:00	17:00	*Extended LAPW method for bulk and semi-infinite crystal calculations*	E. Krasovskii	Kiel
17:00	18:00	*A combined APW-PW scheme for self-consistent calculations*	F. Starrost	Kiel
19:00		**Joint dinner**		

Saturday, Nov 7th, 1998

Morning session:

9:00	9:45	*Implementation of noncollinear magnetism*	L. Nordström	Uppsala
9:45	10:15	*A new way of linearizing the APW-method*	E. Sjöstedt	Uppsala
10.15	11.45	*Exact exchange within the LAPW method*	P. Dudešek	Graz
11.45	12:00	**coffee break**		
12:00	12.30	*Linear response theory within ab-initio bandstructure*	R. Kouba	Graz
12:30	13:00	*Round Table discussion: Nitty-Gritty Details*		
13.00	14.00	**Lunch**		
14:00	14:45	*Application of the FP-LAPW method to the structural analysis of corundum type metal oxide surfaces*	X.-G. Wang	Berlin
14.45	15:30	*Magnetic Surfaces under electric fields*	X. Nie	Jülich
15.30	16:00	*Xe/Ag(001) under electric fields*	S. Clarke	Cardiff
16.00	16.05	**Closing**		

ABSTRACTS:

An Introduction to the FLAPW-7 Program

G. Bihlmayer
IFF, Forschungszentrum Jülich, Germany

Abstract

This talk will give a short introduction to the basic features of our full-potential LAPW program for bulk and film geometry and the improvements made in the last few years. The focus of this contribution will be on the calculation of surfaces and magnetic properties, including the treatment of spin-orbit coupling, external electric fields etc. New algorithmic changes to speed up or refine parts of the calculations will be discussed and a short outlook to future developments will be given.

Xe/Ag(001) under electric fields

Sean Clarke[1], John E. Inglesfield[2], Maziar Nekovee[3], Peter K. de Boer[4]
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[2] *Department of Physics and Astronomy, University of Wales Cardiff, PO Box 913, Cardiff, CF2 3YB, United Kingdom*
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[4] *Department of Physics, University of Nijmegen, Toernooiveld, NL-6525 ED Nijmegen, The Netherlands*

Abstract

FLAPW calculations for the electronic structure of Xe c(2x2)-Ag(001) were performed within the LDA using the embedding method to provide a true semi infinite substrate. These calculations included the application of a static planar electric field to the system, and the effect of this perturbation on the electronic structure of the system was studied yielding results in good agreement with classical estimates for screening. The concept of effective charge was generalised to arbitrary electric fields and a method for obtaining forces without calculating total energies was illustrated using this concept. This concept was then used to make estimates of the forces felt by an Xe atom adsorbed on an Ag(001) substrate in the presence of an applied field and the results were used to make some comment on field desorption experiments and the Eigler atomic switch.

Exact exchange within the LAPW method

P. Dudešek[1], C. Ambrosch-Draxl[1] and A. Görling[2]

[1]*Institut für Theoretische Physik, University Graz, Austria*
[2]*Lehrstuhl für Theoretische Chemie, Technical University München, Germany*

Abstract

Within the Kohn-Sham formalism, exchange and correlation potential and energy are usually treated by the local density approximation (LDA) limiting the accuracy of the results. As a consequence e.g. the unoccupied bands are poorly described leading to underestimated band gaps. It has been shown recently [1] that within the Kohn-Sham procedure not only the exchange energy but also the exchange potential can be treated exactly and therefore only for the electron correlations an approximation is needed. This scheme, which is self-interaction free, has been successfully applied to the pseudopotential method improving the energy gaps of semiconductors [2]. We have worked out the formalism within the LAPW method. Thus, to our knowledge, it will be the first implementation of EXX into an all-electron full-potential method. We construct the EEX potential with the help of the linear response (LR) operator. For numerical reasons, it is not suitable to develop the LR operator within the LAPW basis set. Thus an auxiliary basis set is introduced. The exchange potential cannot be directly added to the effective potential in this form. Hence, the exchange contributions to the Hamilton matrix elements are computed directly. This guarantees that the self-consistency procedure can be carried out then as usual. By applying this method to a variety of solids we expect to gain more insight into the role of exchange and correlation effects for different materials.

[1] A. Goerling, Phys. Rev.B **53** 7024 (1996).

[2] M. Städele, J. A. Majewski, P. Vogl, A. Görling, Phys. Rev. Lett. **79** 2089 (1997).

Linear–response theory within ab–initio bandstructure calculations

R. Kouba
Institute of Theoretical Physics, University Graz, Austria

First, I present various ab–initio techniques to determine the phonon spectra of a solid within bandstructure calculations. Second, I report on our current work to implement one of these techniques, namely the iterative linear–response formalism (Baroni et al,1987), into the WIEN97-program package.

Essentially frequencies and eigenvectors of lattice vibrations can be determined by obtaining total energy and atomic force values at a set of various phonon distorted lattice configurations. This approach requires the performance of bandstructure calculations within supercells, whose dimensions are commensurate with the q–vector of the phonon. Large unit cells increase the computational effort significantly, so that this approach is limited to high symmetry phonons. Alternatively, the phonon vibration can be regarded as a small perturbation to the undistorted lattice so that the dynamical matrix can be obtained on the basis of first–order changes in the self–consistent effective potential and in the electronic charge density. These first–order changes can either be evaluated via the inverse of the dielectric matrix or via an iterative linear-response formalism. Whereas the computational effort in both approaches is widely q–independent, the latter one is more suitable in its adaption to mixed-basis sets (LMTO and LAPW), avoids the direct summation over unoccupied states and does not require the inversion of large response matrices. For these reasons we are implementing the iterative LAPW linear–response formalism (Yu et al.,1994) on an all–electron basis into the WIEN97–program.

Extended LAPW method for bulk and semi-infinite crystal calculations

E. E. Krasovskii

Institut für Theoretische Physik, Universität Kiel, Germany

Abstract

I present the formalism and describe the properties of the extended linear augmented plane wave $\vec{k}\cdot\vec{p}$ method for solving the Schrödinger equation. A distinctive feature of the method is that the relevant matrices (hamiltonian, overlap, and momentum matrices) are computed only once for a given crystal potential, which speeds up the calculation of the electron eigenstates of an infinite crystal. The accuracy of the $\vec{k}\cdot\vec{p}$ method depends upon the extension of the radial basis set. I show the applications of the ELAPW-$\vec{k}\cdot\vec{p}$ method to the calculations of the complex dielectric function of metals $\epsilon(0,0,\vec{q})$ in the long wavelength limit (optical spectra) as well as for finite $\vec{q}$ (plasmon dispersion). The method reduces the inverse bandstructure problem to a matrix eigenvalue problem, which gives access to the electronic structure of a semi-infinite crystal. I present the calculations of the LEED states for (111) surfaces of the fcc metals Cu, Ag, and Al and (0001) surfaces of $1T$ chalcogenides VSe_2 and TiS_2 and compare the theoretical target current spectra with measurements.

Electric fields applied to magnetic surfaces

X. Nie[1], S. Heinze[1], M. Weinert[2], and S. Blügel[1]

[1] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

[2] *Department of Physics, Brookhaven National Laboratory, Upton, NY 11973 U.S.A.*

Abstract

Electric fields at surfaces or interfaces occur in electrochemical environments and by application of the atomic force or scanning tunneling microscope. Until now magnetic surfaces under electric fields are little investigated. We have implemented into our FLAPW-code the spin-orbit interaction in second variation and an external electric field interacting at the surface. Two applications are reported: (i) The change of atomically resolved STM-images from corrugating to anticorrugating images under electric fields, and (ii) the modification of magnetic properties under an electric fields.

Implementation of non-collinear magnetism in the LAPW method

Lars Nordström

Uppsala University, Sweden

Abstract

It is reported how a continuous version of non-collinear magnetism can be implemented in the full-potential linear augmented plane wave method. This implementation has been performed within the framework of both the local spin density and the general gradient approximations of density functional theory. As demonstrations of applications, calculations for three different kinds of non-collinear magnetism were presented.
1) Relativistic effects, i.e. spin orbit induced non-collinearity: fcc Pu.
2) Frustrated antiferromagnetism: fcc Fe.
3) Fermi nesting induced helical ordering: hcp rare earths.
In connection with the last application it was demonstrated how so-called spin spiral symmetry can be used within a full-potential scheme.

Improving the efficiency of FP-LAPW Calculations

Max Petersen, Frank Wagner, Lars Hufnagel, and Matthias Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

Abstract

The *full-potential linearized augmented-plane wave* (FP-LAPW) method is well known to enable most accurate calculations of the electronic structure and magnetic properties of crystals and surfaces. After the implementation of atomic forces [1] the main drawback of the FP-LAPW method, compared to the pseudopotential plane wave (PPW), has been its higher computational expense.

We analysed the FP-LAPW method from a computational point of view. Starting from an existing implementation [2], we identified the time consuming parts and show how some of them can be formulated more efficiently. In this context also the hardware architecture plays a crucial role. The remaining computational effort is mainly determined by the setup and diagonalization of the Hamiltonian matrix. For the latter, two different iterative schemes are compared. The speedup gained by these optimizations are compared to the runtime of the "original" version of the code, and the PPW approach.

[1] B. Kohler, S. Wilke, M. Scheffler, R. Kouba and C. Ambrosch-Draxl, Comp. Phys. Comm **94** 31 (1996).

[2] P. Blaha, K. Schwarz, P. Dufek, and R. Augustyn, `WIEN95` (Technical University, Vienna, 1995); improved and updated UNIX version of the original copyrighted `WIEN`-code

Overview of WIEN97 LAPW-code

K. Schwarz
TU Wien, Theoretical Chemistry, Vienna, Austria

Abstract

During the last 15 years a computer code was developed in our group mainly by P.Blaha. Its latest version is WIEN97 which presently is used worldwide by more than 230 groups.

I present our experience in developing such a program package in collaboration with other groups and illustrate its main features. Several topics will be discussed such as i) method development, ii) computational aspects, iii) features and properties, iv) contributions by other groups, and v) possible collaborations in the future.

A new way of linearizing the APW-method

Elisabeth Sjöstedt, Lars Nordström
Uppsala University, Sweden

Abstract

The LAPW basis set consists of two parts, plane waves in the interstitial and orbital solutions inside the muffin-tin (MT) spheres, which are matched in value and in slope over the MT-boundaries. This yields smooth basis functions, but the matching of derivatives requires a larger number of plane waves and therefore increases the already large secular determinant to be solved.

The method presented here, LAPW$^+$ suggests using local orbitals as complementary basis functions to an energy independent APW basis set. The local orbitals are shown to increase the flexibility of the basis set inside the MT-spheres enough to describe all eigen functions in a range around the linearization energy. As no extra conditions are needed for the derivatives of the basis functions (the APW basis functions and the local orbitals need only to be continuous at the MT-boundary) the LAPW$^+$ method can use a smaller basis set, and still yield the same results as the original LAPW method.

The Augmented Fourier Components Method for Constructing a General-Shape Potential

F. Starrost, E. E. Krasovskii, and W. Schattke
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Abstract

The Augmented Fourier Components (AFC) method is a new method for the treatment of a Coulomb potential of general shape [1] within the LAPW formalism. The AFC method is particularly efficient because it is based on the ELAPW-$\vec{k} \cdot \vec{p}$ method [2]. We divide the valence density into two parts, one of which is expanded in a Fourier series throughout the whole unit cell, ρ^F, while the other one is localized in small spheres surrounding the nuclei, ρ^{MT}. To a good approximation ρ^{MT} can be approximated by its Y_{00} component. The quality of the representation is controlled by the number of Fourier components of the density ρ^F, and the computational effort can be balanced with the desired accuracy. By construction the density is smooth everywhere in the unit cell and the representation of the density is free from unphysical parameters specific to the representation of the wave function. The construction of the potential is straightforward and its convergence can be accelerated by

reassigning the rapidly varying part of the Fourier-filtered density ρ^F near the nuclei to the muffin-tin density ρ^{MT}.

[1] E.E. Krasovskii, F. Starrost, W. Schattke, submitted to Phys. Rev. B.

[2] E.E. Krasovskii, W. Schattke, Phys. Rev. B **56**, 12874 (1997).

Application of FP-LAPW method to the structural analysis of corundum-type metal oxide surfaces

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Abstract

Corundum-type metal oxide surfaces are attracting the interest of many experimental and theoretical researchers because of their importance in many technological applications. But, the surface geometries of the flat surfaces are unclear still and even the surface stoichiometries are not known. Using full-potential linearized augmented plan wave (FP-LAPW) method, we have investigated the structural properties of corundum-type metal oxide (α-Al_2O_3, α-Cr_2O_3 and α-Fe_2O_3) (0001) surfaces, and carefully analyze the electronic and magnetic properties, the surface bonding character and the surface reactivities. Various possible surface terminations are taken into account. For the Cr_2O_3 and Fe_2O_3 surfaces, two geometries are found to be particularly stable under thermal equilibrium: one being terminated by one metal-atom (Cr or Fe) layer and the other by O_3 layer. The relative abundance of these two terminations is controlled by the ambient oxygen partial pressure[1]. For α-Al_2O_3 (0001) surface, Al-terminated surfaces is stable. The metal-atom terminated surfaces exhibit a huge inward relaxation of the topmost layer with a small rotation of the O_3 triangles at the first oxygen layer. The O_3-terminated surfaces also present huge and unusual surface relaxations with a large rotation of the O_3 triangles at the topmost oxygen layer.

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Excitation Spectra from Non-Local Screened Exchange and Model-GW: Implementations in the Bulk FLAPW Code and Applications

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and Erich Wimmer[1]

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Abstract

Providing computational tools for an accurate calculation of optical spectra for solids including semiconductors, transition metals and f-electron systems was the starting point and main objective for the reported program developments. In order to overcome the inadequacy of density functional theory to describe electronic excitations, many body approaches such

as non-local screened exchange (sX-LDA) [1] and model-GW [2] are implemented in the bulk FLAPW code [3]. Also taking into account spin-orbit coupling in second variation, the overall agreement of band gaps, electronic transitions and band positions with experimental data is excellent for group IV, III-V, and II-VI semiconductors. The evaluation of oscillator strengths and the conductivity tensor enables ab-initio predictions for optical spectra of doped III-V semiconductors with engineering quality. Finally, ongoing code development efforts towards efficient geometry optimization, local orbitals as well as elastic and phonon properties are outlined.

[1] D. M. Bylander and L. Kleinman, Phys. Rev. B **41**, 7868 (1990); A. Seidl, A. Görling, P. Vogl, J. A. Majewski,and M. Levy, Phys. Rev. B **53**, 3764 (1996).
[2] F. Gygi, A. Baldereschi, Phys. Rev. Lett. **62**, 2160 (1989); S. Massidda, A. Continenza, M. Posternak, and A. Baldereschi, Phys. Rev. B **55**, 13494 (1997).
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4.1.2 Report on Bogoliubov-de Gennes Workshop

THE VTH BRISTOL WORKSHOP ON THE
BOGOLIUBOV-DE GENNES EQUATIONS

Sponsored by the **CCP9** (UK) and the **TMR2** Network (EU)

Organised by **B L Gyorffy, J F Annett and J Quintanilla**
(University of Bristol)

Burwalls, Bristol, November 20-22, 1998

There was, once again, an increased turn out for this, by now, annual event. As usual there were a number of talks reviewing certain areas. Others reported new developments. For example the Würzburg project of constructing exchange and correlation functionals for superconductors has made significant progress with the incorporation of phonons and, therefore, retarded effective, attractive interaction into the process. The Stuttgart group reported fully tested simple tight-binding model Hamiltonians ready to be used in many-body calculations. The new result from the Daresbury-Bristol collaboration on the quasi-particle spectra of the high $T_c$cuprates were the first calculations of the penetration depth $\lambda(T)$ for YBCO in very satisfactory agreement with the experiments. There was also a report of new insights on the damping of the de Haas-van Alphen oscillations in the superconducting state. Interest in exotic pairing, and not just in the cuprates, were very much in evidence with talks on grain boundary effects, disorder and prospects of new materials. The very interesting contributions of the Lancaster group on coherent transport in superconducting nano-structures was supported by an experimentalists review of the experimental situations.. Given the hope that some day such systems may serve as q-bits in quantum computing we invited Sandu Popescu, a leading figure in this most promising field, to discuss the basic issues to be addressed. Although the bipolaron model lost nothing of its contraversiality it was shown to give rise a most surprisingly simple phenomenological description of the highs and lows of T_c among the high T_c materials. Finally, both the correlations beyond LDA and the break down of the Migdal theorem for the electron-phonon vertex were critically examined and illuminated by new calculations. The final programme is given below and further details of the subjects can be gleaned from the abstracts of talks included below.

Programme

Saturday 21

9:00-9:30 Miguel Marques (Würzburg)

Coulomb correlations in the DFT for superconductors: an LDA for the exchange free energy functional

9:30-10:00 Dzidka Szotek (Daresbury)

The quasi-particle spectrum of YBCO in the superconducting state

10:00-10:30 T. Saha-Dasgupta (Stuttgart)

Tight-binding modelling using 3rd generation LMTO methods

10:30-11:00 I. Dasgupta (Stuttgart)

Trends in LDA-derived model Hamiltonians for cuprate High-Tc Superconductors

11:00-11:15 **COFFEE**

11:15-11:45 Martin Lüders (Würzburg)

How to treat electron-phonon coupling in the DFT for superconductors

11:45-12:30 Sandu Popescu (Cambridge)

Quantum Computing

12:30-1:00 Colin Lambert (Lancaster)

Phase Coherent Transport in Superconducting Nano-structures

1:00-2:00 **LUNCH**

2:00-2:30 Tero Heikkila and Colin Lambert (Lancaster)

Conductance oscillations and fluctuations in Andreev interferometers

2:30-3:00 Rob Seviour (Lancaster)

Conductance suppression in mesoscopic normal-superconducting structures

3:00-3:30 Fabbio Taddei (Lancaster)

Superconductivity and magnetic multilayers

3:30-4:00 Steve Bailey (Lancaster)

The Whispering Gallery modes in mesoscopic normal-superconducting structures

4:00-4:30 **TEA**

4:30-5:00 Lars Fast (Würzburg)

Numerical solutions of the DFT gap equation

5:00-5:30 Jason Hogan-O'Neill and James Annett (Bristol)

Grain-boundary effects in D-wave superconductors

5:30-6:00 Anatoly Volkov (Lancaster)

Methods of quasiclassical Green's functions in the theory of transport in superconducting nanostructures

6:00-6:30 Kevin Duncan (Bristol)

A damping of the de Haas-van Alphen oscillations in the superconducting state

6:30-8:00 **DINNER**

8:00-8:45 A S Alexandrov (Loughborough)

The theory of the superconducting transition temperature in the cuprates

Sunday 22

9:00-9:30 James Annett (Bristol)

Exotic pairing in non-cuprate superconductors

9:30-10:00 Karol I. Wysokinski (Lublin)

D-wave pairing in disordered superconductors

10:00-10:30 Andrew Martin (Geneva)

Localization and D-wave superconductivity

10:30-11:00 Jonathan Wallington (Bristol)

TBA

11:00-11:30 **COFFEE**

11:30-12:00 Victor Petrashov (Royal Holloway College, London)

Coherent electron transport through mesoscopic ferromagnetic superconducting junctions

12:00-12:30 Walter Temmerman (Daresbury)

Self-Interaction Corrected LDA for YBCO

12:30-1:00 Evgenii Maximov (Cambridge)

Non-adiabatic effects in the phonon spectra of normal and superconducting metals

1:00–2:00 **LUNCH**

Abstracts of Talks

A Local Density Approximation For Superconductors

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Abstract

Conventional Density Functional Theory (DFT) is not able to describe the superconducting phase of matter. In 1988, Oliveira, Gross and Kohn [*Phys. Rev. Lett.* **60**, 2430 (1988)] developed the formal framework of a DFT for superconductors. Practical applications of this theory, however, have been rather scarce, mainly due to the fact that first-principles approximations for the exchange-correlation potentials were not available.

In this talk we propose an LDA-type functional describing the electronic correlations of inhomogeneous superconductors. This functional is constructed in analogy to the Local

Spin Density Approximation (LSDA). First one determines the exchange-correlation energy per volume, $f_{\rm xc}^{\rm hom}$, of the homogeneous electron gas exposed to a translationally invariant pairing field. The quantity $f_{\rm xc}^{\rm hom}$, which is a functional of the density n and of the induced order parameter χ, is calculated using many-body perturbation theory. We give explicit expressions for the first-order exchange diagrams and for an RPA-like approximation for the correlation energy. The RPA includes the sum over all the normal and anomalous bubble diagrams. The LDA functional for inhomogeneous systems is then defined by $F_{\rm xc}^{\rm LDA} = \int d^3\mathbf{R} f_{\rm xc}^{\rm hom}[n(\mathbf{R}), \chi_W(\mathbf{R},\mathbf{k}]$, where χ_W is the Wigner transform of the (non-local) order parameter $\chi(\mathbf{r},\mathbf{r}')$ of the inhomogeneous system. The functional reduces to the normal-state LDA in the limit of vanishing order parameter, and a systematic gradient expansion of the total energy functional shows that this is in fact the *only* correct LDA for superconductors.

A Semiphenomenological Approach for Description of Quasiparticles in High Temperature Superconductors

Z. Szotek$^{(a)}$, B. L. Gyorffy$^{(b)}$, W. M. Temmerman$^{(a)}$, O. K. Andersen$^{(c)}$, and O. Jepsen$^{(c)}$
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$^{(c)}$ *Max-Planck-Institut für Festkörperforschung, Postfach 800665, D-70506 Stuttgart, Germany*

Abstract

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

Tight-Binding Hamiltonians from Third-generation LMTO method

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Abstract

We show how the third-generation LMTO method can be employed to obtain first-principles tight-binding Hamiltonians. The advantage of this method, compared to the previous versions is that the new LMTO sets give wave functions which are correct to (ϵ_i - ϵ_ν) (ϵ_i is the single-particle energy obtained from LMTO basis and ϵ_ν is the energy about which linearisation has been performed), not only inside the muffin-tin spheres, but also in the interstitial region. As a consequence, the simple and popular formalism which previously resulted from the atomic-spheres approximation (ASA) now holds in general, that is, it includes downfolding and the combined correction. The power and flexibility of the new method will be demonstrated by deriving few-orbital, low-energy, tight-binding Hamiltonians for the high T_c superconductors and Ladder compounds. Our method being free from any fitting procedure contains the information of the wavefunctions.

Trends in LDA-derived model Hamiltonians for cuprate High T_c Superconductors

I. Dasgupta, O. K. Andersen, O. Jepsen, T. Saha-Dasgupta
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Abstract

We describe the electronic structure of cuprate high temperature superconductors in terms of low energy model Hamiltonians. We discuss the trends, in particular the role of the *minority* apical oxygen p_z , Cu $3z^2-1$ and Cu s orbitals on the LDA conduction band structure of a series of single layer cuprates: La_2CuO_4, $Tl_2Ba_2CuO_6$, $HgBa_2CuO_4$ and $CaCuO_2$. We show that, except for La_2CuO_4, the by-mixing of Cu $3z^2-1$ is negligible and that the apical oxygen p_z can be folded into the Cu-s orbital. This gives rise to a *chemical* Cu x^2-y^2, Cu s, O p -orbital model. From its calculated parameter values the on-site energy of the effective Cu-s orbital is found to be the essential material dependent parameter and is controlled mainly by the position and binding of the apical oxygen when present. The Cu-s orbital also provides the hopping between the oxygens inside the layer, controls the instability towards dimpling and buckling and provides the main channel for hopping perpendicular to the layer $t_\perp(\vec{k}_{||})$. We discuss the the $\vec{k}_{||}$-dependence of $t_\perp$ for the simple tetragonal and the body centered tetragonal cuprates. Finally, we discuss the influence of the effective Cu-s and the geometry of the CuO planes on the stationary points of the conduction band structure which gives rise to Van Hove singularities (VHS) in the densities of states close to the Fermi level. The role of such VHS's on the calculated doping dependence of d-wave superconducting transition temperature (T_c) is discussed.

Density-Functional Theory for Superconductors: How to treat the electron-phonon coupling

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Abstract

A generalization of the density functional theory (DFT) for superconductors is presented which allows the treatment of strong electron-phonon coupling. To this end, a multicomponent DFT for the electron-ion system is established using as basic variables the normal density of the electrons, the anomalous density (i.e. the order parameter of the superconducting state), and the diagonal of the ionic two-particle density matrix. The resulting Kohn-Sham (KS) system consists of non-interacting electrons and of ions interacting with each other but not with the electrons. The KS equation for the ions is then expanded around the ionic equilibrium positions and expressed in terms of KS phonons. The electronic KS Hamiltonian can be diagonalized by the Bogoliubov-Valatin transformation, giving rise to the KS-Bogoliubov-de Gennes equations. These contain, in principle, all electronic correlations as well as correlations mediated by the movement of the ions.

An approximation to the exchange-correlation (xc) functional is obtained by many-body perturbation theory. The unperturbed system consists of non-interacting electrons and non-interacting phonons, while the Coulomb-interaction as well as the electron-phonon interaction is treated as perturbation. For the Coulomb interaction an RPA-type approximation is employed by resumming all normal-state bubble diagrams (in static approximation). The phonon-mediated interaction is taken into account by the first-order diagrams with respect to the full (time-dependent) KS-phonon propagator.

Conductance oscillations and fluctuations in Andreev interferometers

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Abstract

Andreev interferometers are a useful tool for probing the effects of the proximity of superconductors on transport through normal (nonsuperconducting) mesoscopic structures. In these devices, the normal structure is in contact with two superconducting segments with order-parameter phases ϕ_1 and ϕ_2. The conductance through the structure has an oscillatory dependence on the phase difference $\phi = \phi_1 - \phi_2$ and the energy-dependent amplitude of these oscillations measures the difference between strong ($\phi = 0$) and weak ($\phi = \pi$) proximity effects. The behaviour of the conductance yields an insight on the properties of Andreev reflection.

In this talk a few of the main findings concerning the Andreev interferometers will be pointed out, such as the reentrant energy dependence and the suppression of zero-phase

conductance in the presence of tunnel barriers. The interpretation of these effects will also be discussed shortly.

I will also report on the results of our numerical simulations based on the Bogoliubov-de Gennes equation on a tight-binding lattice. These include the geometry dependence of the conductance oscillation amplitude (behaviour of the amplitude as the distance between the superconductors is increased) and the superconductivity-induced suppression of universal conductance fluctuations.

Conductance suppression in mesoscopic normal-superconducting structures

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Abstract

Experiments on hybrid superconducting normal-metal (S/N) structures have revealed that the onset of superconductivity can lead to a decrease in the electrical conductance by an amount many orders of magnitude greater than e^2/h. In the absence of tunnel barriers we provide a theory of this phenomenon which shows that it originates from an instability in the 4 - probe conductance which is absent from 2-probe measurements.We compare the zero-bias, zero-temperature 4-probe conductances G_N and G_S of a normal diffusive metal in contact with a superconductor in both the normal (N) and superconducting (S) states respectively. In the absence of tunnel barriers, the ensemble average of the difference $\delta G = G_S - G_N$ vanishes, in agreement with quasi-classical theory. However we also predict that there exists macroscopic sample specific fluctuations in δG, which lie beyond quasi-classical theory and allow large negative values of δG to occur.

In addition, using a scattering matrix approach and quasiclassical Green's function technique, we calculate the conductance of 2 probe S/N structures consisting of a superconductor in contact with normal diffusive wire where an effective barrier between the superconductor and the normal wire exists. We establish that the difference between the superconducting and normal state conductance ($\delta G = G_s - G_n$) is negative for large S/N interface resistances ($R_{S/N}$) and changes sign with decreasing $R_{S/N}$.

Superconductivity and magnetic multilayers

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Abstract

In this paper we examine the interplay between ferromagnetism and superconductivity in magnetic multilayers exhibiting giant magnetoresistance (GMR). The structure considered consists of a sequence of alternating non-magnetic and magnetic layers with a normal contact at one end and a superconducting contact at the other. The magnetizations of the magnetic layers are either parallel (P) or antiparallel (AP) to each other and the current flows perpendicular to the plane of the layers.

When the energy of the electrons carrying the current is below the superconducting energy gap Δ, no transmission is allowed into the superconductor. Therefore the electrons impinging on the superconductor are reflected back into the magnetic structure either as electrons with the same spin or as holes with opposite spin (Andreev reflection).

Our study is based on a numerical solution of the Bogoliubov-de Gennes equation for clean magnetic multilayers described with an $s-p-d$, material dependent, tight-binding Hamiltonian. The conductance is evaluated using a multiple-scattering formalism for the two spin fluids. The magnetic and non-magnetic metals considered in the study are, respectively, Co and Cu, Ag, Pt. We find that the conductance is always decreased by the presence of the superconductor in the P configuration and not much affected in the AP configuration. This leads to a suppression of the GMR, which, for some non-magnetic material thicknesses, can even take negative values.

Effective interaction kernel in the DFT gap equation

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Abstract

Density functional theory (DFT) for superconducters provides a set of Bogoliubov-type Kohn-Sham equations. In the vicinity of T_c, these equations can be linearized leading to a gap equation which rigorously determines the critical temperature T_c. The interaction kernel entering this linearized gap equation is given by the second functional derivative of the exchange-correlation (xc) free energy with respect to the order parameter, evaluated at vanishing order parameter. For the phonon mediated part of the xc functional we use the Eliashberg-type diagrams presented in the talk by M. Lüders. The purely electronic correlations are approximated by an RPA for the *inhomogeneous* system. Explicit results, for the interaction kernel are presented for aluminium. It turns out that the RPA effective interaction is nearly constant in the first Brillouin zone. The divergence of the bare Coulomb interaction at $k = k'$ is strongly screened. Numerical solutions of the gap equation are presented. In order to investigate the dependence of T_c on the large-k behavior (which is very hard to determine from the band structure) of the effective interaction we have also employed simple model functions for the interaction kernel.

The Whispering Gallery Modes in Mesoscopic Normal-Superconducting Structures

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Abstract

Recent experiments by Mota et al. [1] on superconducting wires such as Niobium coated by a normal metal such as Silver, reveal suppression of the proximity effect at low temperatures. It has been suggested [2] that this originates from the prescence of sub-gap **Whispering Gallery** modes which are associated with the cylindrical geometry of the samples. In this paper, we compute the density of quasi-particle states of a superconducting circle embedded in a normal annulus and compare this with a corresponding sample of square geometry. We find that the circular sample does indeed possess low lying peaks in the density of states which are absent in the square sample. These peaks are destroyed by both disorder and applied magnetic field but are resistant to surface roughness and slits in the normal annulus.

1. R. Franssanito, P. Visani, M. Niderost and A.C. Mota; P. Smeibidl, K. Swieca, W. Wendler and F. Pobell, Czech. Journal of Physics, **46** (1996) S4.
2. Christoph Bruder and Yoseph Imry, Phys. Rev. Lett. **80**, 5782 (1998).

Symmetric and Non-symmetric Superconducting Grain-Boundaries: a Self-Consistent S- and D-wave study

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Abstract

Grain-boundaries are important weak-link junctions in high T_c superconductors. Previously the study of interfaces in superconductors has been confined to flat interfaces or 90^o twin boundaries, and have relied upon k-space calculations. Here we use a more realistic model, butting together two squares lattices at an angle of misorientation , θ. We find two general classes of boundary, symmetric and non-symmetric. For such systems we self-consistently solve the Bogoliubov-de Gennes equations using the Recursion Method for both s- and d-wave superconductors. Our real space method calculates how the superconducting order parameters, charge densities, and local densities of states are affected by the boundary. In a d-wave system we find an induced extended-s component at the boundary. By imposing phase differences in either order parameter across the boundary we present self-consistent profiles of current versus phase and find a saw-tooth profile with a step at $+/-\pi$. This step can be attributed to a sudden filling-in of the energy gap at this phase difference. In the symmetric junction we do not find broken time reversal symmetry.

Methods of quasiclassical Green's functions in the theory of transport in superconducting nanostructures

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and Physics Department, Lancaster University, Lancaster, UK

Abstract

A brief introduction to a method of matrix Green's functions (the Keldysh technique) is given in the report. We show how this method can be used to describe transport in mesoscopic $S/N/S$ structures. Using this method we obtain results which explain the oscillatory behaviour of the conductance G of $S/N/S$ structures in a magnetic field and a nonmonotonic dependence of G on temperature. We also discuss the stationary Josephson effect in nonequilibrium $S/N/S$ structures and the possibility to obtain negative Josephson coupling energy (pi-contact).

A Damping of the de Haas-van Alphen Oscillations in the superconducting state

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Abstract

We have developed a semiclassical theory in the superconducting state and study the de Haas-van Alphen oscillations. We find that the oscillations have the same frequency as in the normal state but their amplitude is reduced. We argue that the mechanism of damping is tunnelling between semiclassical quasi-particle orbits which have both particle-like and hole-like segments. The quantitative predictions of the theory are consistent with the available data.

Superconducting T$_c$ in cuprates

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Abstract

Based on the exact cluster diagonalisation and recent Quantum Monte Carlo simulations we analyse the dynamic properties of small polarons and bipolarons formed by a short-range (Holstein) and long-range (Fröhlich) electron-phonon interaction. We show that the exact results agree well with the canonical Holstein theory for a cluster and with the Lang-Firsov theory for a lattice. For a long-range interaction the Lang-Firsov theory of a single polaron and our $1/\lambda$ perturbation expansion in a multi-polaron system are almost exact in a wide range of the adiabatic parameter ω/t including the intermediate regime. The polaron and bipolaron bandwidth is not necessary small and the damping effects are negligible at temperatures well below the characteristic phonon frequency. We show that recent claims by several authors with regards to the breakdown of the Holstein-Lang-Firsov theory and 'impossibility' of bipolaronic superconductivity are the result of of an erroneous interpretation of the electronic and vibronic energy levels of a two-site Holstein model, misunderstanding of the perturbation theory and the electron-phonon interaction in ionic solids with polaronic carriers. The (by)polaron theory, when properly applied, agrees well with the numerical results and provides a parameter-free expression for the superconducting critical temperature of layered cuprates.

Exotic pairing in non-cuprate superconductors

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Abstract

Unconvneitonal pairing (p or d-wave) is now known to occur in the high T_c cuprate and heavy fermion superconductors. The unusual pairing state suggests novel pairing mechanisms, and may also be related to other 'anomalous' normal state effects such as heavy fermion behaviour, magnetic fluctuations or the normal state pseudogap. It is therefore interesting to ask whether other classes of superconductors also may have p or d-wave pairing states. Indeed there is now strong evidence for p wave pairing in Sr_2RuO_4, and some indications of possible d wave pairing in some organic superconductors. In this talk I shall sumarises some of the evidence for or against p or d-wave pairing in various anomalous systems including the various oxides (especially the ruthenates and the bismuthates) organics,fullerenes, boro-carbides, and other systems such as the C15s.

'D - wave' pairing in Disordered Superconductors.*

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Abstract

A Coherent Potential Approximation is developed for d–wave superconductivity in disordered systems. We show that the CPA formalism reproduces the standard pair-breaking formula, the self-consistent Born Approximation and the self-consistent T-matrix approximation in the appropriate limits. We implement the theory and compute T_c for s–wave and d–wave pairing using an attractive nearest neighbour Hubbard model featuring both binary alloy disorder and a uniform distribution of scattering site potentials. We determine the density of states and examine its consequences for low temperature heat capacity. We find that our results are in qualitative agreement with measurements on Zn doped YBCO superconductors.

(*) *The abstract of the talk delivered by K.I. Wysokiński during the* V^{th} *Bristol Workshop on the Bogolubov – de Gennes Equations held in Burwalls, Bristol, November 20-22,1998 and sponsored by the CCP9 (UK) and TMR (EU) programmes.*

Localization in d–wave superconductors

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Abstract

In this talk I presented a method for determining whether either quasi-particles or Cooper Pairs are localised. This is done by claculating whether a quasi-particle, or Cooper Pair has a finite probability of being on a given site i after infinite time, given that it was on site i with probabiltity 1 at $t = 0$.

Using this as a measure of localization I considered a simple problem, where I had a 2D lattice with a d-wave order parameter and introduced a random set of normal impurity potentials. Solving the Bogoliubov de Gennes Equations, non-self-consistently, for such a system I could determine whether the quasi-particles and/or the Cooper pairs were localised. What I found is certainly for low disorder strengths both the quasi-particles and the Cooper Pairs were not localized, but as I went to higher disorders the low energy quasi-particle states were localized.

Also discussed was whether the local particle density of states, for a d–wave superconductor, is finite at the Fermi energy when disorder is introduced. This point was raised to consider the contoversy surrounding recent, exact analytical, results obtained by A.A. Nersesyan and A.M. Tsvelik which suggest, in contrast to results obtained through the Coherent

Potential Approximation (CPA), that no matter how strong the normal impurity disorder in a d-wave superconductor, the local particle density of states is zero at the Fermi Energy. Through my numerical results for the local particle density of states I found, in agreement with CPA, that the local particle density of states becomes finite upon the introduction of disorder. This raises the dilemma that in both my numerical calculations and A .A. Nersesyan and A.M. Tsvelik analytical results all diagrams are summed over, but we obtain fundamentally different results for the local particle density of states at the Fermi Energy.

Effective field theories for s- and d-wave superconductors

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Abstract

Starting with a microscopic theory of interacting electrons in 2D (extended Hubbard model with nearest neighbour attractive interaction, V) we derive effective bosonic theories to describe s- and d-wave superconductivity.

At the level of mean field (Landau) theory, we find Tc for both channels as a function of band-filling, n, and intercation strength, V. Allowing the order parameters to interact, we see that, as the filling is increased, the system passes from d-wave to (s+id) to s-wave via 2nd order transitions. No mixed (s+d) phase is observed and nor are there any 1st order transitions (s $leftarrowrightarrow$ d).

To allow for the inclusion of fluctuation effects we introduce a weak coupling bewteen 2D planes. When this is done we are able to observe the transition from BCS to Bose-Einstein-type superconductivity. The latter occurs at low densities and high interaction strengths. The nature of the Bose fluctuations changes interestingly with temperature: at low temperatures the fluctuations are quantum mechanical but at high temperatures they are classical. Due to the weak inter-plane coupling, we find that the transition occurs via an intermediate state where the fluctuations are quantum in the planes but the coupling between the planes is incoherent (classical).

Coherent electron transport through mesoscopic ferromagnetic/superconducting junctions

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Abstract

A giant drop in the resistance of diffusive ferromagnetic (F) wires has been observed at the onset of superconductivity of adjacent superconductors with strikingly long-range influence of the latter [1]. The quasiclassical theory [2] does not explain the experiments. A

phenomenological analysis of the results is presented. The conductance, $G_{FN} = 1/R_{FN}$, of the F-wire at zero temperature can be written in terms of numbers of spin-up, $n_{\uparrow}$, and spin-down, $n_{\downarrow}$, conduction channels in the bandwidth of Thouless energy $G_{FN} = \frac{e^2}{h}(n_{\uparrow} + n_{\downarrow})$. For a finite temperature, L should be substituted with appropriate kinetic coherence length, ξ_{kin}, with $R_{FN} = \frac{\rho_F \xi_{kin}}{w d_F}$. When the adjacent N-metal goes superconducting, the contributions to the conductance of the channels are enhanced by a certain factor, η, varying in the range $1 < \eta < 2$. Then G_{FS} becomes $G_{FS} = 2\eta \frac{e^2}{h} n_{\downarrow}$ with the change in the resistance at the onset of superconductivity, $\frac{\Delta R_{FS}}{R_{FN}} = 1 - \frac{1}{\eta(1-P)}$, where $P = \mid \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}} \mid$ is the spin polarization, changing sign at $\eta = \frac{1}{(1-P)}$. The character of the dV/dI curves for F-wires [1,3] suggests that the value of η depends on the energy of the quasiparticles leading to the crossover from $\Delta R_{FS} > 0$ to $\Delta R_{FS} < 0$ [3]. The lower bound for the coherence length is estimated $\xi_{kin} = 0.2 \mu m$ which is more than two orders in magnitude larger than the "thermodynamic" coherence length ξ_m.

1. V. T. Petrashov, I. A. Sosnin, I. Cox, A. Parsons, and C. Troadec, submitted to PRL (1998).
2. C.J. Lambert and R. Raimondi, J. Phys. Condens. Matter **10**, 901 (1998).
3. V.T. Petrashov, V.N. Antonov, S. Maksimov, and R. Shaikhaidarov, JETP Lett. **59**, 551 (1994); M. Giroud, H. Courtois, K. Hasselbach, D. Mailly, and B. Pannetier, Phys. Rev. B **58**, 11872 (1998).

Self-Interaction Corrected LDA for YBCO

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Abstract

It is well-known that the Local-Spin-Density Approximation (LSDA) cannot describe the antiferromagnetic groundstate for La_2CuO_4 and $YBa_2Cu_3O_6$[1]. However, the application of the self-interaction-corrected (SIC) LSDA to La_2CuO_4 leads however to the correct anti-ferromagnetic groundstate [2]. In this contribution we will show that the SIC applied to $YBa_2Cu_3O_6$ also leads to an anti-ferromagnetic groundstate. This we obtain by applying the SIC to the Cu orbitals in the CuO_2 planes and in the CuO chain. For the Cu orbitals in the plane, nine orbitals are subjected to the SIC, namely, the five majority spin orbitals and in the minority channel the three t_{2g} and of the e_g's the d_{3z^2-1}. For the Cu orbitals in the chain, we apply the SIC to all ten orbitals. In this contribution we also discuss the implications of these results for the description of the electronic structure of $YBa_2Cu_3O_7$.

1. W.M. Temmerman, H. Winter, Z. Szotek and G.Y. Guo, Physica B **172** 279 (1991)
2. A. Svane, Phys. Rev. Lett. **68** 1900 (1992); W.M. Temmerman, Z. Szotek and H. Winter, Phys. Rev. B **47** 11533 (1993)

Nonadiabatic effects in phonon spectra of normal and superconducting metals

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Abstract

Nonadiabatic contribution of the electron-phonon interaction to the phonon self-energy is studied for normal and supercinducting states of metals for different values of the phonon momentum q.The combined approach is used for invesigations based on the use of the Froulich hamiltonian with parameters calculated in DFT for rigid lattice. It is demostrated that the long-range Coulomb fields does not affect the nonadiabatic phenomenon.It is shown that for the normal state the nonadiabatic effects are important only for optical phonons with small values of the phonon momenta.The results of the theoretical calculations of the renormalization of a phonon frequency and a phonon linewidth is compared with the experimental data on the metal Os.

It is shown in the frame work of the BSC theory that the vertex corrections for q equal zero lead to the appearence of the pole in the phonon self-energy and additional phonon line .The phonon self energy has the logarithmic singularity at large values of q instead of the the square root tipe as at q=0 .It is shown that at q=Q where Q is the nesting vector the phonon self-energy has the same tipe singularity as for q=0.The results are compared with the recent neutron scattering measurements in borocarbides.

5 News from the ESF Programme

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

STRUC-Ψ_k

5.1 Progress Report for 1998

The aim of the Ψ_k-Research Programme of the ESF is to promote the development and application of computational techniques aimed at an improved understanding of the complex atomistic behaviour of solids and surfaces. A characteristic feature of the techniques we are developing is the all interatomic forces and electronic properties are calculated quantum mechanically from first principles. Applications of this techniques are not restricted to condensed matter theory, surface science and materials science, but are rapidly expanding into chemistry, mineralogy and even biology. The efficiency of the computer codes is now sufficient to attack problem of immediate industrial relevance, e.g. in the fields of catalysis, magnetic information storage. The Ψ_k-Research Programme intends to create a scientific network covering all of Europe with connections to groups in the US and in Japan, and with strong links to experimentalists and industry in the expanding range of applications. This networking activity is based on (a) a bimonthly electronic Ψ_k-Newletter, (b) research workshops, (c) hands-on workshops for disseminating computer-codes, (d) collaborative visits and secondments.

The work of the Ψ_k Research Programme was started in June 1998 with a workshop on "Electronic Structure Calculations for Industry and Basic Sciences" at the Technical University of Wien, organized conjointly with the TMR-Network "*Electronic Structure Calculating of Materials Properties and Processes for Industry and Basic Sciences*". The aim of this workshop was to confront the expectations of industrial research with the resources offered by academic research groups in the Ψ_k community. Eight invited speakers from industry described possible areas where computational modelling could be particularly helpful, ranging from the development of catalysts over the electronic and optical properties of pigments and the quality of silicon wafers for microelectronic devices to magnetic materials (again with a wide span from permanent magnets to thin magnetic layers for magnetooptic recording applications). It is expected that this first industry workshop will be followed within the next years by a series of topical meetings confronting industrial and academic research in certain selected areas.

This "Ψ_k-Industry Workshop" was also the occasion for the first meeting of the STRUC-Ψ_k Steering Committee. The Steering Committee approved the appointment of a Core Steering Group that will take care of the administration of the daily business of the workshop and established the budget for the year 1998. Guidelines for the financial support of workshops and collaborative visits were established.

The research workshops organized in 1998 by members of the Ψ_k-Network are listed in Table 1 of the appendix. Detailed reports on all workshops (including complete lists of participants and abstracts of all talks) are published in the Ψ_k-Newletter. For the TB-LMTO workshop, a proceedings volume will be published by Springer. As the particular highlights of the topics discussed in the workshops one should mention the methodological developments discussed in the Lyon and Ste. Odile workshops, the connections to a broad range of materials-science problems discussed in the workshops in Vienna, Il Ciocco and Cagliar, and the applications to mineralogy forming the topic of the Plön workshop. The quest for techniques scaling linearly with the number of atoms ("O(N) techniques") and hence allowing to treat problems of increasing complexity will certainly remain in the focus of the Ψ_k-Research Programme for many years. Wide wide variety of approaches being adopted emphasizes the need for an intense scientific exchange until the optimal strategy for achieving this goal emerges. The topics of the "Nanotechnology" workshop held in Il Ciocco illustrate the widening range of applications of ab-initio techniques stretching to nanoscale-manipulations of atoms at surfaces, to molecular electronics and to catalysis. The "Mineralogy" workshop held in Plön highlights the impact of quantum-mechanical calculations on areas ranging for crystallography to geophysics.

In addition, the Steering Committe decided to support a number of collaborative visits (further applications being approved by the Core Steering Group), see Table 2 in the Appendix. The topics of the collaborations demonstrate the success of the Ψ_k-Research Programm in promoting the further developments of the computational tools, in disseminating the successful methodologies, and in combining the expertise in computation with that in applications in various fields. Reports on these activities are published in the Ψ_k-Newletter. It is expected that the exchanges through collaborative visits and secondments will be intensified in the following years.

The Steering Committee also discussed some projects for 1999 and the organization of a large $\Psi - k$-Conference in the year 2000, the budget for the next year will be elaborate in the meeting of the Core Steering Group on October 24 in Paris.

Jürgen Hafner
(Acting Chairman)

Table 1: **Research Workshops within the Ψ_k Research Programme in 1998**

Workshop (Organizers)	Location (Date)	Co-organized with
Electronic Structure Calculations for Industry and Basic Sciences (J.Hafner, W.Temmermann (Ψ_k), E. Wimmer, A. Svane (TMR)	Vienna June 3-4	TMR "Electronic Structure"
Local Orbitals for Large Scale Atomistic Simulations (D. Pettifor (Ψ_k, P. Ordejón, L. Seijo, G. Galli)	Lyon July 22-25	CECAM
Computational Materials Science (P. Ruggerone, V. Fiorentini (Ψ_k))	Santa Margarita Sept. 18-22	U Cagliari
Properties of Inorganic Crystals from Theory and Experiment (B. Winkler, K. Knorr (Ψ_k), V. Milman (MSI))	Plön Sept. 26 - Oct. 1st	Deutsche Ges. f. Kristallogr., MSI
Computational Physics for Nanotechnologies (A. Fisher (Ψ_k))	Il Ciocco Sept. 19-24	EURESCO
Tight-Binding LMTO Method (H. Dreyssé (Ψ_k and TMR))	Ste. Odile Oct. 2-5	TMR "Interface Magnetism"

Table 2: **Collaborative visits and secondments within the Ψ_k-Programme**

Visitor	Host	Research Topic	Duration (days)
A. Lichtenstein (FZ Jülich, D))	K. Kunc (U Paris VI, F)	Electr. structure and lattice of manganite perovskites	5
A. Postnikov (U Osnabrück, D)	M. Alouani (U Strasbourg, F)	Properties of RENiO$_3$ perovskites	5
E. Wachowicz (U Wroclaw, PL)	C. Stampfl (FHI Berlin, D)	Electronic and structural properties of hcp metals	14
R. Kucharczyk (U Wroclaw, PL)	J. Pollmann (U Münster, D)	Surfaces and interfaces of semiconductors	28
S. Razee (U Warwick, GB)	L. Szunyogh (CMS Wien, A)	Magnetic anisotropy of thin films and multilayers	12
A. Zupan (U Ljubljana, SL)	P. Blaha (TU Wien, A)	Exchange-correlation functionals	5
R. Schmidt (U Frankfurt/M., D)	K. Schwarz (TU Wien, A)	Relativistic local orbitals in FLAPW	5
W. Hofer (CMS Wien, A)	S. Blügel (FZ Jülich, D)	Scanning tunneling microscopy simulations	2
K. Kadas (TU Budapest, H)	J. Hafner (CMS Wien, A)	Reconstruction of BN surfaces	28

5.2 Reports on Collaborative Visits

Report on a visit of Elwira Wachowicz (Wrocław, Poland) to Professor Matthias Scheffler's group (Fritz-Haber-Institut, MPG, Berlin)
September 7-19, 1998

I am a Ph.D. student working with Prof. Adam Kiejna (University of Wrocław, Poland) on the properties of close packed hcp metals surfaces (Mg, Be). I use fhi96md code developed by Professor Scheffler's group and the purpose of the visit was to get better understanding of advantages and disadvantages of the code as well as discussing some technical details and difficulties with getting correct results.

In Berlin I worked closely with Dr. Catherine Stampfl. We were trying to understand the reason why the results for Mg bulk properties I had obtained before in Wrocław (lattice constant and c/a ratio) differed significantly from the experimental values. To find out the cause of these discrepancies I did several tests of dependence of input parameters on a calculated total energy. First tests concerned the choice of the cut off energy. After comparing results for cut off energies of the range 10-50 Ry it showed up the 15 Ry is high enough for the convergence of the total energy. Another test examined the choice of the k-points in the irreducible part of the Brillouin zone. The conclusion of such calculations was the big importance of the number of k points. Our results showed reasonable agreement with experimental values for not less than 60 k-points. As the last test I calculated the cohesion energy which was in good agreement with both experimental and achieved by other ab initio calculations values.

Besides, I had a chance to discuss with Dr. C. Stampfl and other members of the group: difficulties with calculating bulk modulus, importance of comparison between LDA and GGA method, choice of the parameters for calculating surface properties and some other problems connected with first principles calculations of hcp metals.

Summarizing, it was very fruitful visit for me and all my plans were fulfilled. It will contribute greatly to the progress in my work in Wrocław.

(Elwira Wachowicz)

Report on the collaborative visit of W. Hofer (CMS Vienna) to Jülich
10–12 September, 1998

I am a PhD student of Dr. J. Redinger at the Technical University of Vienna (Austria) working on the simulation of STM-images of metal surfaces with special emphasis on binary alloys. I visited the group of Dr. S. Blügel at the Institut für Festkörperforschung, Forschungzentrum Jülich (Germany) from September 10 to September 12, 1998. My reasearch entails the development of a numerical scheme to calculate the tunnel currents between the STM tip and the sample surface within Bardeen's transfer Hamiltonian method. I discussed details of the implementation based on the film-FLAPW method and realistic tip models with Stefan Heinze, a PhD student of Dr. Blügels group, and with Stefan Blügel. Of particular concern was the formulation of the tunneling current and the computational speed with which this tunneling current calculation can be performed. We discussed a far-distance approximation valid for realistic tip-sample distance which increases the speed-up by 2 order of magnitudes. The performance of a preliminary implementation has been tested on a T90. This visit has complimented earlier activities of Weinberger and Blügel and was important to set up a longer collaboration on the problem of calculating STM-currents within FLAPW.

(W. Hofer)

5.3 Reports on Workshops

5.3.1 Report on Workshop in Plön

Report on the workshop
'Structures and Properties of inorganic crystals from theory and experiment'
Plön, Germany, 26.09-01.10.1998

This report concerns a workshop on 'Structures and properties of inorganic crystals from theory and experiment', held in Plön, FRG, from the 26.09-01.10.1998. The workshop was funded in the framework of the ESF Programme 'Electronic structure calculations for elucidating the complex atomistic behaviour of solids and surfaces'. It was organised by B. Winkler, (University Kiel), V. Milman (MSI, Cambridge) and K. Knorr (Hahn-Meitner-Institute, Berlin). 25 participants from eleven European countries attended. The participants were coming from industry, research institutes and universities.

The aim of the workshop was to bring together experimentalists from the chemistry, mineralogy, physics and material science communities with researchers developing and applying quantum mechanical codes to establish the extent to which parameter-free calculations can be used to support experimental investigations. There were six lectures per day, addressing (i) general capabilities of modern quantum mechanical programs, (ii) physics of phonons, (iii) study of surface properties, especially related to catalysis, and (iv) the analysis of electron densities. About half of the lectures were devoted to experimental studies, such as coherent inelastic neutron scattering, resonant ultrasound spectroscopy, nuclear magnetic resonance, SPM techniques and others. This allowed to critically analyze the accuracy, precision, and effort of modelling studies and the insight they provide with respect to experimental investigations. Specifically for the interpretation of spectroscopic measurements of complex, low symmetry structures reliable parameter-free models would be very helpful, as was demonstrated in several talks on phonon measurements and calculations. Discussions also centered around the limits of current ab initio techniques with respect to system size, and the use of empirical and semi-empirical methods as complementary modelling techniques.

The extended abstracts have been collected as a booklet, an online-version is available at `http://www.min.uni-kiel.de/kristallographie/esf/seite1.html`. There, a list of participants and further information can be found as well. The discussions were very lively and sometimes controversial, continuing throughout meals. The conference center in Plön provided a pleasant surrounding. Computers were provided by the Institute for Mineralogy in Kiel, and several test calculations with different software packages (SIESTA, CASTEP, GULP and others) were undertaken during the workshop.

In summary, from the organisers point of view this has been a very succesful meeting, contributing to a mutual education between experimentalists and modellers. Several collaborations were started at the workshop. Of course, this meeting would not have been possible without the finacial support by the ESF, for which we are very grateful.

B. Winkler, V. Milman, K. Knorr

5.3.2 Report on Meeting on Nanostructures

MEETING REPORT
COMPUTATIONAL PHYSICS FOR NANOTECHNOLOGY
A.J. Fisher

The European Research Conference on 'Computational Physics for Nanotechnology' took place at the Il Ciocco conference centre, Castelvecchio Pascoli, Tuscany, Italy from 19 to 24 September. About 60 researchers from 17 countries spent five agreeable days in the Tuscan hills discussing how the techniques of modern electronic structure theory can help to address some of the crucial issues in nanotechnology, enjoying the view, and sampling the wonderful food.

The meeting was supported by the ESF (through the Euroconferences programme and through the network 'Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces'), by the UK Engineering and Physical Sciences Research Council, and by the Thin Films and Surfaces Group of the Institute of Physics. The meeting was part of the more-or-less official series on the Electronic Structure of Solids which began in Cambridge in 1992.

Sessions addressed both the new types of calculations that will be needed for nanotechnological applications, and some of the pioneering calculations that have already been performed. The sessions on computational methods included talks on the calculation of excitation energies within density functional theory (by E.K.U. Gross), on $O(N)$ *ab initio* electronic structure techniques (by D.R. Bowler), on the incorporation calculation of nuclear wavefunctions for surface chemical reactions (by A. Gross) and on the need of a wide variety of computational tools for technological applications (E. Wimmer). A session on charge transfer processes (with talks by W.M. Schmickler, U. Peskin and J. Ulstrup) stressed the challenge of incorporating inelastic and solvent-related effects into dynamical descriptions of phenomena such as surface electron transfer.

Organic materials have a found number of novel applications in nanoscale systems, and talks by G. Brocks and S. Stafström focussed on calculations of the electronic properties of such systems. Inorganic materials also pose considerable computational challenges on the nanoscale, and the meeting heard talks by J.-L. Martins, F. Buda, R. Perez, A. Williamson and I. Stich on systems as diverse as diamond polishing, clusters, magnetic films, zeolites, and quantum dots. The interface between electronic structure and many-body physics in quantum dots was highlighted by H. Bruus. Finally, there were several talks on probe microscopy and the properties of the truly atomic-scale structures that can be produced by this technique; once again, the coupling of electrons to other degrees of freedom featured in the contributions from J. Hoekstra, K. Jacobsen, L. Pizzagalli and J.-L. Mozos.

We departed with a feeling of great excitement at the challenges and opportunities offered to computational physicists in this field, and a renewed awareness of the many different physical phenomena needed for a successful description of nanoscale systems.

The next meeting in the series, on chemical reactions at surfaces, will be chaired by Axel Gross (Munich) in 1999. At the 1998 meeting we had to choose a chair and a conference topic for 2001, and Philip Lindan (Daresbury) was elected to chair a conference on simulations of complex surface and interfacial processes. Both promise to be very exciting meetings.

5.4 Workshop/Conference Announcements

5.4.1 High Pressure Workshop in Daresbury

WORKSHOP ON MATERIALS UNDER PRESSURE: FROM ICES TO METALS

Daresbury Laboratory (UK) 17–18 December 1998

Supported by **CCP9**: Computational Studies of Electronic Structure of Solids
and **ESF** Programme Psi-k: Electronic Structure Calculations for elucidating
the complex atomistic behaviour of solids and surfaces

Organized by Richard Nelmes and Walter Temmerman
(rjn01@isise.rl.ac.uk or w.m.temmerman@dl.ac.uk)

SCOPE

Recent experimental developments on synchrotrons and neutron facilities have led to much improved structural studies of materials under pressure. Simultaneously, more accuracy in the band structure studies of materials have allowed to explore the crystal structure under pressure in greater detail. The aim of this workshop is to increase the dialogue between experimentalists and theoreticians.

PROVISIONAL PROGRAMME

Thursday 17 December 1998

10:00 10:30 Coffee

10:30 11:15 Review Talk Metals (Theory): Borje Johansson (Uppsala)
11:15 11:45 Discussion

11:45 12:15 Rajeev Ahuja (Uppsala)

Structural Phase Transitions in Alkali metals, Alkaline earth metals and Alkali Hydrides and Halides.

12:15 12:30 Discussion

12:30 14:00 Lunch

14:00 15:45 Review Talk Metals (Experiment): Malcolm McMahon (Edinburgh)

14:45 15:15 Discussion

15:15 15:45 Metals Talk (Experiment): Andrew Jephcoat (Oxford)

15:45 16:00 Discussion

16:00 16:30 Coffee

16:30 17:00 Metals Talk (Theory): Axel Svane (Aarhus)

17:00 17:15 Discussion

17:15 17:45 Karl Syassen (Stuttgart)

New crystal structures of elemental metals under pressure

17:45 18:00 Discussion

18:00 19:00 Visit to SR

19:30 Conference Dinner

Friday 18 December 1998

9:00 9:45 Dominik Marx (Stuttgart)

Ab Initio Simulations of Materials under High Pressure

9:45 10:15 Discussion

10:15 10:45 Stewart Clark (Durham)

High pressure structure of methanol and ethanol

10:45 11:00 Discussion

11:00 11:30 Coffee

11:30 12:15 John Finney (UCL)

Structures, disorder, and metastability in ices at medium pressures

12:15 12:45 Discussion

12:45 13:45 Lunch

13:45 14:30 Talk (Experiment): John Loveday (RAL)

14:30 14:45 Discussion

14:45 15:15 Martin Dove (Cambridge)

High-pressure behavior of minerals

15:15 15:30 Discussion

15:30 16:00 David Sherman (Bristol)

Chemical bonding and Electronic transitions in the Earth's Deep interior

16:00 16:15 Discussion

16:15 Coffee and End of Workshop

EUROPEAN RESEARCH CONFERENCE on Electronic Structure of Solids and Surfaces: Challenges in predictive descriptions of reaction dynamics and growth properties at surfaces

Sept. 18-23, 1999, Hotel Arabella Brauneck, Lengries, Germany

Supported by:
The Programme of European Research Conferences (EURESCO)
Psi-k Euro-Network for Electronic Structure Calculations

Chairperson:	Axel Groß (TU München, Germany)
Vice-Chairpersons:	Gianfranco Pacchioni (Universitá Milano, Italy)
	Thorsten Klüner (FHI Berlin, Germany)

The last five years have seen a tremendous step forward in the understanding of the interaction of molecules with surfaces. The next great challenge is the description of more complex reactions and processes on surfaces. The first crucial step to investigate reactions theoretically is the evaluation of the potential energy surface on which the reaction takes place. But equally important are dynamical simulations on these potential energy surfaces to actually obtain reaction rates and probabilities.

The main goal of this conference is thus to address the questions, what are the relevant degrees of freedom for the treatment of reaction dynamics and growth properties at surfaces, how does one get a reliable description of the interaction potentials, and how should one perform the dynamical simulation of these processes. Although the main focus of this conference rests on theoretical methods, the participation of experimentalists and industrialists is considered to be most important.

The invited speakers who have confirmed their participation include the following:

- General concepts of density-functional theory and reactivity theories
  - Axel D. Becke (Kingston, Canada)
  - E.J. Baerends (Amsterdam, NL)
  - Rex W. Godby (York, UK)
  - Bjørk Hammer (Aalborg, DK)
- Analytical or numerical representation of the potential energy surface (PES)
  - Doug J. Doren (Newark, USA)
  - Horia Metiu (Santa Barbara, USA)
- High-dimensional quantum dynamics and dissipative dynamics
  - Geert-Jan Kroes (Leiden, NL)
  - Didier Lemoine (Lille, France)
  - Ronny Kosloff (Jerusalem, Israel)
  - Shiwu Gao (Göteborg, Sweden)
- Catalysis and biochemical reactions
  - Dave A. King (Cambridge, UK)
  - Jens K. Nørskov (Lyngby, Denmark)
  - Notker Rösch (M"unchen, Germany)
- Growth and etching, corrosion and lubrication
  - Talat S. Rahman (Kansas, USA)
  - Anne M. Chaka (Lubrizol Corp., USA)
- Electronically non-adiabatic and collision and photo-induced effects
  - John C. Tully (New Haven, USA)
  - Peter Saalfrank (Berlin, Germany)
  - Mario Rocca (Genova, Italy)
  - Katharina Al-Shamery (Berlin, Germany)

Further information is available at:
http://www.physik.tu-muenchen.de/lehrstuehle/T30g/Conf/erc_lengries.html

5.4.3 Programme of Psi-k Workshops in 1999

ESF-Programme Sponsored Psi-k Workshops for 1999

1. **Calculation of Material Properties using Total Energy and Force Methods and ab initio Molecular Dynamics**, Trieste, August 9 - 18, 1999
Organized by Peter Kratzer, Jörg Neugebauer and Matthias Scheffler (all at Fritz-Haber-Institut, Berlin, Germany) and by Jorge Kohanoff (International Centre for Theoretical Physics, Trieste, Italy)
The workshop will give an introduction and hands-on training of density functional theory and the pseudopotential/plane-wave method. Accordingly the focus of the workshop will be on practical exercises at a PC or computer terminal. We plan to give both lectures and extensive tutorials on the various aspects of using the plane-wave computer code developed at the Fritz-Haber-Institut. In addition, the participants will get an introduction to various important aspects related to the plane-wave total-energy calculations, like the construction of ab initio pseudopotentials, the treatment of excited states, performing molecular dynamics calculations, and other simulation techniques based on the total energies obtained with the plane-wave method. Apart from the practical exercises, we will arrange lectures by invited experts which will explain both the basic architecture of the computer code, but will also cover the more fundamental background of density functional theory. For further information, see
http://www.fhi-berlin.mpg.de/th/Meetings/trieste.html
http://www.ictp.trieste.it/www_users/calendar/cal1999.html
For questions, send e-mail to fhiwrk@fhi-berlin.mpg.de.

2. **Progress in Computational Materials Science**, Strasbourg, June 1-4, 1999
Computer modeling is of importance in materials science in two ways. First, it can be a means of calculating the consequences of basic theories, in which the main goal is to gain a qualitative understanding of trends and relations. Secondly, modeling can also be used as an "experimental" technique, where the aim is to accurately describe a specific material or process. Both approaches are extremely valuable and will be addressed at the proposed meeting. This symposium intends to bring together researchers from a wide range of subfields in computational materials science. The aim is to discuss common trends and problems, but also to produce cross-fertilization between disciplines. The emphasis will be on genuine materials problems, studied in a realistic way, and on systems or processes of actual industrial or technological importance. New algorithms and implementations as well as novel theories are welcome provided they have the potential of applicability to real-world problems. Materials of interest range over metals and semiconductors (as well as their alloys), oxides, polymers, glasses, composites, and biological systems. These may be composed as small clusters or nanoparticles, or may be in bulk form. Of equal relevance are surface and interface phenomena, including multilayers and thin films. Amorphous systems and liquids are also within the scope of this symposium.Phenomena to be covered include: electronic structure and its macroscopic effects; magnetism, particularly in films and multilayers; cluster assembly, cluster deposition, and irradiated solids; mechanical

properties, such as fracture, dislocations, stress, etc.;growth and evolution of thin films and other microstructures; thermodynamics and kinetics of phase transformations, including metastable phases and systems far from equilibrium. Particular attention will be given to the following issues: relating the electronic structure of materials to simulation parameters; comparing and contrasting ab-initio and semi-empirical approaches; methods for going beyond the local density and Born-Oppenheimer approximations; addressing the relation between atomic and continuum models; describing algorithms for parallel and other high-performance computers, in particular O(N) methods; new developments in Monte Carlo, molecular dynamics, and other simulation techniques.

3. **Challenges in predictive descriptions of reaction dynamics and growth properties at surfaces**; Lengries, Germany; September 18-23, 1999. Organised by Axel Groß (TU München, Germany), Gianfranco Pachioni (Universitá Milano, Italy) and Thorsten Klüner (FHI Berlin, Germany).

The last five years have seen a tremendous step forward in the understanding of the interaction of molecules with surfaces. Due to advances in density functional theory algorithms and an increased effort in the dynamical simulation of processes on surfaces the paradigm for simple reactions on surfaces – the dissociation of hydrogen on metal surfaces – seems to be understood to a large extent now. The next great challenge is the description of more complex reactions and processes on surfaces. The study of these reactions is important for a wide range of applications as heterogeneous catalysis, corrosion or passivation of surfaces, lubrication, growth properties for building better devices, the hydrogen storage in metals, just to name a few. The first crucial step to investigate reactions theoretically is the evaluation of the potential energy surface on which the reaction takes place. But equally important are dynamical simulations on these potential energy surfaces to actually obtain reaction rates and probabilities. The main goal of this conference is thus to address the questions, what are the relevant degrees of freedom for the treatment of reaction dynamics and growth properties at surfaces, how does one get a reliable description of the interaction potentials, and how should one perform the dynamical simulation of these processes. These research subjects are really multi-disciplinary. This conference should therefore appeal to experts from the fields of surface science, chemistry, biochemistry, material science, and statistics. Although the main focus of this conference rests on theoretical methods, the participation of experimentalists and industrialists is considered to be most important since the detailed information that modern theoretical and experimental tools can give about surface processes allows a close and fruitful collaboration.

For further information, see
http://www.physik.tu-muenchen.de/lehrstuehle/T30g/Conf/erc_lengries.html

4. **Magnetism and Magnetoanisotropy of Surfaces and Interfaces** Riksgransen, Sweden, May 1999. Organised by Lars Nordstrom, Jurgen Henk and Olle Eriksson, Uppsala University, Sweden

This will be a three/four day workshop with focus on longer invited lectures of prominent researchers in the fields of magnetism of surfaces and interfaces. In addition to the more educational part of the workshop there will be a few oral contributions, but most contributions will be presented in poster sessions. The scope of the conference will cover theoretical and experimental aspects of thin film magnetism. Special emphasis will be put on magnetoanisotropy; spin and orbital magnetism; magnetostrictive effects; magneto recording phenomena (magneto optical effect and GMR); effects of temperature; structural effects; interface roughness.

5. **Catalysis from First Principles,** Copenhagen, May 17-19, 1999
The objective of the meeting is to review the status of electronic structure and total energy calculations as a basis for an understanding of chemical reactions on solid surfaces. A strong focus will be placed on the prosects of calculational methods becoming a tool in the design of newcatalysts. An additional objective in this connection is to bring together researchers from the electronic structure community with researchers from experimental surface science and catalysis from academia and industry.

6. **Magnetic Moments of Actinides,** Daresbury Laboratory, June 4-5, 1999
The magnetism of transition metal systems and lanthanide systems is now fairly well understood, where d and f electrons can be described in a delocalized and localized model, respectively. On the other hand, actinide systems do not fit in such a description. The localization of the 5f is in between that of the 3d and 4f and the strong spin-orbit interaction necessitates a relativistic approach. Furthermore, electron correlation effects play a major role in these compounds. Recently, it has become possible to determine element- specific magnetic moments using neutron diffraction and x-ray scattering and absorption. The latter technique makes it even possible to separate the orbital and spin contribution to the total magnetic moment. The results are very interesting but difficult to reproduce with present state-of-art calculations. Not only a very large orbital polarization but also a large magnetic dipole term has been measured in cubic compounds, such as US. This allows for severe testing of the extra terms included in band theory to account for orbital polarization. It is also clear that deeper insight in magnetism can be obtained by studying the unusual behaviour of the actinides. Despite the fact that actinides for health reasons will find less application in technological market products, the understanding of their magnetic and electronic properties will no doubt provide key elements for a general description of electron correlation and relativistic effects.

7. **Workshop on Computational Materials Science, Magnetic Moments of Actinides,** Sardinia September 1999
This workshop aims to focus on the application of ab initio approaches to the real-life problems posed by experiment and by technologically relevant phenomena. Therefore, the meeting will also cover, without neglecting the first principles "soul", reviews of experimental aspects, and of alternative methods. For example, semiempirical approaches, Monte Carlo simulations, Tight-Binding Molecular Dynamics, with the goal being to show how theory can bridge microscopic aspects with meso- and macroscopic time and length scale. More specifically, a session will be centered on new aspects related to density functional theory in order to give a overview on the last progresses in first principle methods. Applications will be reviewed The talks are also expected to touch on "exotic" aspects described and handled by ab initio methods, but implemented in different approaches, as e.g path integrals. For example: biological systems, photonic crystals, solids under extreme pressure, etc. More "traditional" applications cannot be neglected. Recent advances in surface and interface physics, and in the physics of ferroelectric phase transitions will be discussed General reviews on simulations and statistical mechanics

models applied to material science will be given. Further, one or two experimental talks will be selected among recent advances in fields to be determined later.

8. **Hydrogen Defects in Semiconductors,** Exeter April 15-16 1999
This workshop brings together modellers, experimentalists and industrialists studying hydrogen related phenomena in semiconductors. There is a great deal of interest in the behaviour of hydrogen in these materials. In addition to passivating donors and acceptors, activating other centres which are inert without the presence of hydrogen, enhancing oxygen diffusion, and exhibiting tunnelling phenomena, hydrogen raises fundamental questions about the accuracy and scope of theoretical modelling methods. The workshop will include invited talks from leading researchers in the field. See http:*//newton.ex.ac.uk/research/theory/jones/hydrogen/* for further details.

6 General Job Announcements

Position of "Assistant-Doctorant" at the EPF-Lausanne

The Institute for Numerical Research in the Physics of Materials (IRRMA) at the EPFL in Lausanne is seeking an outstanding PhD student to perform research in the domain of first-principles electronic structure calculations and quantum molecular dynamics simulations. The position requires a universitary degree in physics or physical chemistry (or equivalent), which should have been obtained by the starting date, i.e. April 1st 1999. The candidate will have teaching duties and shall prepare a doctoral thesis at EPFL. A good background in quantum mechanics and previous experience in FORTRAN programming are required. The interested candidates should send by January 15th, 1999. their (1) curriculum vitae, (2) the list of passed examinations and relative marks, and (3) confidential letters of recommendation to **Dr. Alfredo Pasquarello, IRRMA-EPFL, PPH-Ecublens, CH-1015 Lausanne, Switzerland, Tel. +41/21/6934416, email: Alfredo.Pasquarello@epfl.ch.**

Postdoctoral Position in Condensed Matter Theory, University of Uppsala, Sweden

One or two post-doctoral positions are available in the area of electronic structure theory of solids from January 1999. The positions are available for one year and may be extended for one more year. The main aim of the project is to perform atomistic simulations of technologically important systems such as hard materials, ductile materials, Solar energy materials and magneto-optic materials. First principles calculations, based on density functional theory (in combination with accurate total energy methods: FPLMTO and FPLAPW) and molecular dynamics simulation, will be used.

Applicants should have, or expect soon to obtain, a PhD in Physics or Chemistry, with experience in computational condensed matter theory. Interested persons should send their resumes and the names of references as soon as possible.

Dr. O. Eriksson, olle.eriksoon@fysik.uu.se, Tel: +46 18 471 3625
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Postdoctoral Position in Solid State Theory Group

National Renewable Energy Laboratory

http://www.sst.nrel.gov

The Solid State Theory Group at the National Renewable Energy Laboratory invites applications for a postdoctoral research position to start in the summer or fall of 1999. Applications are accepted now. The position is for two years, renewable upon mutual agreement to a third year, and is in the area of development of electronic structure theory, algorithms and applications to nanostructures and alloys. The Solid State Theory Group currently consists of ten Ph.D.'s in condensed matter theory and interacts with a broad range of experimentalists at NREL. The group has outstanding computational facilities, an excellent basic-research atmosphere, and is located near the beautiful Rocky Mountains. For more information about the group research activities, publications and personel, see http://www.sst.nrel.gov. Interested candidates should immediately send in writing (no e-mail submission) a curriculum vitae, list of publications (including preprints of unpublished papers, if possible) and should arrange for 2-3 reference letters to be sent directly to:

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

NREL is an equal opportunity/affirmative action employer.

Postdoctoral Position in Condensed Matter Theory Group

North Carolina State University

A postdoc and/or a senior postdoc position has recently become available with the Condensed Matter Theory group at North Carolina State University, beginning this Fall or Spring. Our main activities are centered on the application and development of electronic structure methods. Specific projects concern nanotube materials, wide gap semiconductors, and semiconductor surface problems. The primary tool of investigation is the real-space multigrid method implemented on massively parallel supercomputers. The ab initio calculations are complemented with classical Molecular Dynamics and kinetic Monte Carlo simulations as needed.

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

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

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

Jerry Bernholc
E-mail: bernholc@ncsu.edu
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Chris Roland
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NC State Univ., Raleigh, NC 27695-8202
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SENIOR RESEARCH SCIENTIST

DARESBURY LABORATORY, CHESHIRE, UK

The Computational Materials Science group at CLRC Daresbury Laboratory is seeking to fill a staff position concerned with the theory of surface spectroscopy and diffraction. The successful candidate will work within an internationally recognised team of scientists to develop the theoretical framework and computational tools for the interpretation of various photon and electron scattering experiments at surfaces. This work will be performed in collaboration with leading academic research groups in the United Kingdom. There will also be an opportunity to work closely with researchers performing experiments on the synchrotron radiation source at Daresbury.

Candidates should have a good degree at Ph.D. level and a strong research track record in theoretical surface science or a related discipline. A strong background in advanced scientific computing and experience of collaborative software development is also desirable. For further information contact: **n.harrison@dl.ac.uk or http://www.dci.clrc.ac.uk/Group/DCICSECMG**. The salary range is between 18120 & 31400 GBP (1998 pay award pending). Progression within the salary range is dependent upon performance. A non-contributory pension scheme, flexible working hours and a generous leave allowance are also offered.

Application forms can be obtained from: **Recruitment Office, Personnel Division, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX. Telephone (01235) 445435 (answerphone) quoting reference VN1719/98**. More information about CLRC is available from CCLRC's World Wide Web pages at: **http://www.cclrc.ac.uk**. All applications must be returned by 11 December 1998.

The CCLRC is committed to Equal Opportunities and to achieving the Investors In People standard. A no smoking policy is in operation.

7 Abstracts

Generalized stacking fault energetics and dislocation properties: compact vs. spread unit dislocation structures in TiAl and CuAu.

Oleg N. Mryasov[1], Yu. N. Gornostyrev[1,2] and A.J. Freeman[1]
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Abstract

We present a general scheme for analyzing the structure and mobility of dislocations based on solutions of the Peierls-Nabarro model with a two component displacement field and restoring forces determined from the ab-initio generalized stacking fault energetics (ie., the so-called γ-surface). The approach is used to investigate dislocations in $L1_0$ TiAl and CuAu; predicted differences in the unit dislocation properties are explicitly related with features of the γ-surface geometry. A unified description of compact, spread and split dislocation cores is provided with an important characteristic "dissociation path" revealed by this highly tractable scheme.

(Accepted to Phys. Rev. November 1998)
Manuscript available from: onm@saturn.phys.nwu.edu and
www.pluto.phys.nwu.edu/ onm

Ab initio theory of the interlayer exchange coupling

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Abstract

Ab initio formulations of the interlayer exchange coupling (IEC) between two, in general non-collinearly aligned magnetic slabs embedded in a non-magnetic spacer are reviewed whereby both the spacer and the magnetic slabs as well as their interfaces may be either ideal or random. These formulations are based on the spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method, the Lloyd formulation of the IEC, and the coherent potential approximation using the vertex-cancellation theorem. We also present an effective method for the study of the temperature dependence of the IEC. The periods, amplitudes, and phases are studied in terms of discrete Fourier transformations, the asymptotic behavior of the IEC is briefly discussed within the stationary-phase method. Numerical results illustrating the theory are presented.

(Proceedings of the TMR workshop on the TB-LMTO method, 2–5 October 1998, Mont Saint Odile, France, to be published in 'Lecture Notes in Physics' (Springer Verlag))
Postscript file available from: kudrnov@fzu.cz

Temperature dependence of the interlayer exchange coupling in magnetic multilayers: ab-initio approach

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Abstract

The temperature dependence of interlayer exchange coupling (IEC) is studied theoretically on an *ab initio* level using the spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method and the Lloyd formulation of the IEC. We develop an efficient method for calculating integrals involving the Fermi-Dirac distribution by representing the occurring integrands by a sum of complex exponentials. Once the weights of the complex exponentials are determined, the IEC for any given temperature can be evaluated. The results of such calculations agree with results of a direct approach using a complex contour integration with a few Matsubara frequences enclosed. Application is made to Co/Cu/Co(001) trilayers with varying thicknesses of the spacer, and for different thicknesses of the magnetic layers. In the limit of large spacer thickness the present results confirm that the temperature dependence of the IEC is of the form $cNT/\sinh(cNT)$, where T is the temperature and N is the spacer thickness, as predicted by theoretical considerations. The combined effect of the temperature and the disorder in the spacer is also discussed.

(Submitted to Physical Review B)
Latex file and postscript files of figures available from: drchal@fzu.cz

Disordered Alloys and Their Surfaces: The Coherent Potential Approximation

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Abstract

A recently developed *ab initio* approach to the electronic structure of substitutionally disordered alloys and their surfaces is reviewed. It is based on (i) the tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic sphere approximation which provides a physically transparent solution of the one-electron problem in metallic materials, (ii) the coherent potential approximation (CPA) for a mean-field treatment of the substitutional randomness, and (iii) the surface Green functions for a proper description of the true semi-infinite geometry of surfaces and interfaces. Theoretical formulation of fundamental electronic quantities, both site-diagonal (charge densities, densities of states) and site non-diagonal (the Bloch spectral functions) is presented. Transformation properties of the LMTO-CPA theory as well as specific problems of application of the local density approximation to random alloys are briefly discussed and basic algorithms employed in the numerical implementation of the formalism are described.

(Proceedings of the TMR workshop on the TB-LMTO method, 2–5 October 1998, Mont Saint Odile, France, to be published in 'Lecture Notes in Physics' (Springer Verlag))
Postscript file available from: turek@ipm.cz

Ab-initio molecular dynamics studies of the graphitization of flat and stepped diamond (111) surfaces

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Abstract

We present *ab-initio* molecular dynamics studies of the graphitization of flat and stepped diamond (111) surfaces. The fully selfconsistent calculations were performed within the local-density functional approximation with ultrasoft pseudopotentials and periodic boundary conditions. We investigated the effects of the system size, heating rate and other computational parameters. We observe a graphitization (within some ps) of the clean diamond (111) surface only at very high temperatures of 4000 K. A step on the surface has no significant influence on the graphitization temperature when the Pandey chains of the (2×1) reconstructed surface are running parallel to the step. But if this is not the case, i.e. if the reconstruction has a rotated domain, the graphitization temperature is lowered to 2500 K.

(Physical Review B, in print)
Preprints available from: jhafner@tph.tuwien.ac.at

Structural, electronic and magnetic properties of nickel surfaces

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Abstract

The structural, electronic and magnetic properties of the low-index surfaces of Nickel have been investigated via fully self-consistent *ab-initio* local-spin-density-functional (LSDF) calculations. Our technique is based on ultrasoft pseudopotentials, residuum minimization techniques for the calculation of the electronic ground-state and of the Hellmann-Feynman forces and stresses, and on a conjugate-gradient technique for the optimization of the atomic structure. The calculations were performed for nine-layer symmetric slabs, allowing for the relaxation of the upper three layers. We also present a detailed analysis of electronic surface states.

(Surface Science, in print)
Preprints available from: jhafner@tph.tuwien.ac.at

Coherent epitaxy and magnetism of fcc-Fe films on Cu(100)

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Abstract

The epitaxy of face-centred-cubic (fcc) Fe layers on a Cu(001) substrate has been investigated by *ab initio* local-spin-density calculations (including generalized gradient corrections) as a function of the thickness of the film. Fe films with a thickness varying between one and three monolayers (ML) adopt a ferromagnetic (FM) ground-state. For thicker films with an even number of Fe layers (4 ML, 6 ML and 8 ML) a bilayer antiferromagnetic (AF) structure develops, while for an odd number of Fe layers (5 ML, 7 ML and 9 ML) a variety of energetically almost generate spin-structures with a ferromagnetically coupled bilayer at the free surface are found. The magnetic structure of the films is strongly coupled to their crystal structure: the interlayer distance between ferromagnetically coupled layers is expanded, that between antiferromagnetically coupled layers is reduced compared to the layer-distance in the substrate and in ideal fcc Fe films. Our results explain the observed change from a tetragonally distorted structure in the ferromagnetic regime to thicker films that are almost fcc (on average) due to the antiferromagnetism in the deeper layers.

(J. Phys.: Condens. Matter, in print)

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

Metal-insulator transition in approximants to icosahedral AlPdRe

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Abstract

The electronic structure of icosahedral Al-Pd-Re alloys has been calculated for a series of large approximants. For the 1/1 to 3/2 approximants with up to 2292 atoms/cell the electronic eigenstates have been calculated selfconsistently via diagonalization of the Hamiltonian in a tight-binding linear-muffin-tin orbital representation. For the 5/3 and 8/5 approximants only the total and partial densities of states have been calculated using the real-space recursion method. The electronic structure of Al-Pd-Re differs from that of other icosahedral phases by (i) the appearence of a semiconducting gap for certain approximants and (ii) by a scaling behaviour of the participation ratio of the states close to the Fermi level, indicating a critical character of the eigenstates. Our results for the electronic structure are discussed in connection with the outstanding physical properties of icosahedral Al-Pd-Re alloys, and in particular with the possible occurence of a metal-insulator transition in this material.

(Submitted to Phys. Rev. B)
Preprints available from: jhafner@tph.tuwien.ac.at

Ab-initio calculations of the atomic and electronic structure of diamond (111) surfaces with steps

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Abstract

We present *ab-initio* local-density functional calculations of the atomic and electronic structure of stepped diamond (111) surfaces. The relaxation of an ideal monoatomic step with bulk-terminated terraces results in sp^2 bonding near the step. The spacing between the surface layers is also increased. A (2 × 1) reconstruction of the terraces lowers the surface energy and decreases the distance between the first two bilayers, but the step energy is increased. As on the flat (111) surface, hydrogen stabilizes the unreconstructed (1 × 1) surface on the terraces. The carbon atoms at the edge of the step have two dangling bonds. As the energy gained by forming an extra C–H bond is larger than the step-formation energy, exposure of C(111) to atomic hydrogen can lead to a roughening of the surface. The local electronic structure close to the step has been investigated.

(Physical Review B **56**, 2161 (1998))
Preprints available from: jhafner@tph.tuwien.ac.at

Hydrogen adsorption on palladium: a comparative theoretical study of different surfaces

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Abstract

The interaction of atomic hydrogen with the Pd(111), Pd(100) and Pd(110) surfaces is studied by ab initio density functional calculations within the generalized gradient approximation (GGA). For the three surfaces we have determined the prefered adsorption sites, the adsorption structures, the work function changes and the surface diffusion barrier including relaxation effects. This comparative study allows to see some common features, in particular in the adsorption energies and geometries for both surface and subsurface H-atoms, and some significant differences such as the surface diffusion and the dispersion of the H-induced surface state. The origin of these differences is explained by a detailed analysis of the electronic structures of both clean and hydrogen-covered surfaces. Our study leads to an interesting correlation between the hydrogen diffusion barrier and the surface roughness since it plays a important part in the catalytic activity of the respective surfaces.

(Surface Science **411**, 1223 (1998))
Preprints available from: jhafner@tph.tuwien.ac.at

Local order in liquid potassium-antimony alloys studied by neutron scattering and ab-initio molecular dynamics

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Abstract

The structure and chemical bonding properties of liquid K-Sb alloys have been investigated using neutron scattering experiments and ab-initio molecular dynamics simulations. For alloys containing between 25 and 50 at.pct. Sb, the neutron data demonstrate the existence of a well defined prepeak a Q∼ 1.15 Å reflecting a pronounced short-range order. The ab-initio calculations show that the chemical bonding obeys a generalized Zintl-principle, i.e. a formally complete electron transfer from K to Sb. The liquid structure is determined for the "octet" composition K_3Sb by charge ordering effects leading to a salt-like atomic arrangement, at the equiatomic composition by the formation of short covalently bonded Sb-chains in close analogy to the isoelectronic chalcogen elements in the liquid state.

(Europhysics Letters **43**, 539 (1998))
Preprints available from: jhafner@tph.tuwien.ac.at

Structure and Magnetic Properties of thin Mn/Cu(001) and CuMn/Cu(100)films

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Abstract

The structure and magnetic properties of Mn and CuMn overlayers on Cu(001) are investigated within the generalized-gradient approximation of density-funtional theory via *ab initio* calculations based on the ultrasoft pseudopotential method. For a one monolayer (1 ML) Mn-film we predict in-plane $c(2\times2)$ antiferromagnetism with large moments, a slight outward relaxation and almost no buckling. For a 2 ML Mn-film we find layered antiferromagnetism, a modest outward relaxation of both overlayers and again no buckling. For a $c(2 \times 2)$ 1 ML CuMn surface alloy we find a high-moment (m_{Mn}=4.09 μ_B) ferromagnetic ground-state with a pronounced buckling of 0.26 Å . A $c(2\times2)$ 2 ML CuMn alloy-film is antiferromagnetic (m_{Mn_1}=4.13 μ_B and m_{Mn_2}=-3.66 μ_B in the first and second layer,respectively), with strong outward relaxation and buckling of the top layer. The surface alloy is found to be energetically more favourable than an overlayer. The predicted relaxation and buckling are shown to be driven by magnetic effects. It is shown that the strong enhancement of the magnetic moments in the surface alloy is also reflected in a large exchange splitting in the Mn-*d* band.

(Surface Science Letters, in print)
Preprints available from: jhafner@tph.tuwien.ac.at

Ab-initio studies of polyanionic clustering in liquid alloys

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Abstract

The formation of polyanionic clusters in alloys of alkali metals with polyvalent elements has been studied using ab-initio local-density-functional techniques. Tetrahedral Sn_4^{4-} polyanions have been identified in crystalline and liquid KSn, whereas the clusters existing in crystalline NaSn are largely destroyed on melting. Chain-like polyanions are found in crystalline and liquid KSb and in Te-rich K_xTe_{1-x} ($x \sim 0.12$) alloys, Te-dimers are formed in equiatomic KTe, both in the solid and liquid phases.

(Proceedings of the 10th Intern. Conference on Liquid and Amorphous Metals,
J. Non-Cryst. Solids, in print)
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Isolated magnetic moments in icosahedral Al-Pd-Mn alloys

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Abstract

We present ab-initio calculations of the formation of magnetic moments in a large approximant to icoshedral Al-Pd-Mn quasicrystals. It is shown that large magnetic moments can form on a small number of Mn-sites characterized by a loose coordination by Al-atoms and some close Pd-neighbours. d-d hybridization is shown to play an important role.

(Physical Review B, in print)
Preprints available from: jhafner@tph.tuwien.ac.at

Adsorption of CO on Rh(100) studied by ab-initio local-density-functional calculations

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Abstract

Ab-initio local-density-functional studies of the adsorption of CO on the (100) surface of Rh have been performed. We show that although adsorption in the bridge-site is always energetically more favourable than adsorption in either the on-top or the hollow sites, two different mechanisms can lead to a relatively high occupation of the on-top sites: (i) At higher coverage the interactions between the adsorbates stabilize a pseudo-hexagonal coincidence lattice with the experimentally observed $p(4\sqrt{2} \times \sqrt{2})$ structure with a bridge/on-top ratio of 2:1 (all adsorbates being slightly shifted from their high-symmetry positions). (ii) At lower coverages there seems to be a contradiction between the energetic preference for bridge-site adsorption and the mixed top/bridge adsorption reported in the experiments. This could simply be dismissed as a failure of density-functional theory. However, we speculate about a possible way to reconcile the calculated potential energy surface and the experimental observations: At distances larger than 1.75 Åfrom the surface (this is smaller than the equilibrium height for on-top adsorption), the interaction-energy with the on-top site is always larger by $\sim$ 0.5 eV than with the bridge-site. The on-top adsorbed molecule is metastable, because there is a barrier of 0.06 eV for migration to the bridge site and the reaction channel is very narrow. This leads to the observed mixed occupation of top and bridge sites at lower coverage ($\Theta \leq 0.5$).

(J. Chem. Phys. **109**, 5585 (1998))
Preprints available from: jhafner@tph.tuwien.ac.at

Polyanionic and octet-phases in the K-Sb system
I. Crystalline intermetallic compounds

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Abstract

The crystal structure, chemical bonding and electronic properties of intermetallic compounds in the K-Sb system have been investigated using first-principle-local-density-functional calculations including generalised gradient corrections. It is shown that the chemical bonding obeys a generalised Zintl-principle, i.e. a formally complete electron transfer from K to Sb. The stable crystal structure is determined for the stoichiometric octet compound K_3Sb by the formation of an ionic lattice, at the equiatomic composition by the formation of covalently bonded Sb_∞^--helices in close analogy to the isoelectronic chalcogen elements. At intermediate compositions the Sb atoms cluster together to form chain-like polyanion radicals, the electrons provided by the excess alkali metal serving to partially saturate the dangling bonds at the chain ends. It is demonstrated that density functional theory describes the crystal structure of all compounds with high accuracy. The over-binding characteristic of the local density approximation is most pronounced in the alkali-rich limit, but merely causes a scaling of all interatomic distances without distorting the structure. Gradient corrections substantially improve the prediction at large K-content, but tend to overshoot in the Sb-rich range.

(Physical Review B, in print)
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Polyanionic and octet-phases in the K-Sb system
II. Liquid alloys

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Abstract

The structural, dynamic and electronic properties of liquid K_3Sb and KSb alloys have been investigated using ab-initio density functional molecular dynamics. We demonstrate that as for the corresponding crystalline compounds the chemical bonding is determined by a generalised Zintl-principle. Consequently, the local order in the liquid is similar to that in the crystalline phases: At the octet composition the dominant feature is Coulombic charge-ordering. At the covalent equiatomic composition the Sb-atoms share valence electrons in polyanionic clusters forming short, entangled Sb-chains. The $pp\sigma$-bonds stabilising the clusters in the liquid and the helical Sb_∞-chains in crystalline KSb possess considerable flexibility. Therefore, the electronic structure of crystalline and liquid alloys (and consequently their physico-chemical properties) are very similar, although the local order is considerably blurred in the melt.

(Physical Review B, in print)
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Effect of the cluster size in modeling the H_2 desorption and dissociative adsorption on Si(001)

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Abstract

Three different clusters, Si_9H_{12}, $Si_{15}H_{16}$, and $Si_{21}H_{20}$, are used in density-functional theory calculations in conjunction with *ab initio* pseudopotentials to study how the energetics of H_2 dissociative adsorption on and associative desorption from Si(001) depends on the cluster size. The results are compared to five-layer slab calculations using the same pseudopotentials and high quality plane-wave basis set. Several exchange-correlation functionals are employed. Our analysis suggests that the smaller clusters generally overestimate the activation barriers and reaction energy. The $Si_{21}H_{20}$ cluster, however, is found to predict reaction energetics, with $E_a^{\rm des} = 56 \pm 3$ kcal/mol (2.4 ± 0.1 eV), reasonably close (though still different) to that obtained from the slab calculations. Differences in the calculated activation energies are discussed in relation to the efficiency of clusters to describe the properties of the clean Si(001)-2×1 surface.

(Submitted to Phys. Rev. B (June 1998).)
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Density-functional theory studies on microscopic processes of GaAs growth

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Abstract

Results for the elementary processes of MBE growth of GaAs on the frequently used GaAs(001) substrate are reviewed. We propose a bottom-up approach, where a growth model is constructed from the results of density-functional theory calculations. The implications of such a model can be tested against the information from STM images. First the stable surface reconstructions are reviewed. Under the most commonly used conditions for MBE growth, the arsenic-rich $\beta2$ (2×4) reconstruction, which contains As dimers as basic building blocks, is the most stable. Next, the adsorption and diffusion of Ga atoms and As molecules on this surface is described. The DFT calculations support the picture that adsorbed Ga atoms are quite stable against re-evaporation. Their mobility thus determines the homogeneity of the growing layer. Incorporation of Ga atoms proceeds by splitting the As dimers. We propose a model where growth proceeds in two stages: the filling of trenches in the $\beta2$ (2×4) reconstruction, followed by nucleation of islands on the surface regions where the trenches are filled. We demonstrate how clusters of incorporated Ga atoms act as nuclei for the process of trench filling. Concerning island formation, the role of step formation energies and attachment probabilities of mobile adatoms at steps is discussed. Knowledge of these is crucial for an understanding of island shapes. Ongoing research is aiming at an understanding of the microscopic mechanisms giving rise to the transition between the step-flow mode and the island-nucleation mode of growth.

(Submitted to Progress in Surf. Sci. (July 1998).)
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Ab initio based tight-binding Hamiltonian for the dissociation of molecules at surfaces

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Abstract

A tight-binding total-energy (TBTE) method has been developed to interpolate between first-principles results describing the dissociation of molecules at surfaces. The TBTE scheme requires only a relatively small number of *ab initio* energies as input and gives a reliable global representation of the *ab initio* potential energy surface to within 0.1 eV accuracy compared to the *ab initio* results. This approach will open the way to the *ab initio* molecular dynamics description of reactions invoking many atoms and long time-scales that are currently not accessible by first-principles methods.

(Submitted to Phys. Rev. Lett. (July 1998).)

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Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory.

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Abstract

The package `fhi98PP` allows one to generate norm-conserving pseudopotentials adapted to density-functional theory total-energy calculations for a multitude of elements throughout the periodic table, including first-row and transition metal elements. The package also facilitates a first assessment of the pseudopotentials' transferability, either in semilocal or fully separable form, by means of simple tests carried out for the free atom. Various parameterizations of the local-density approximation and the generalized gradient approximation for exchange and correlation are implemented.

(Submitted to Comput. Phys. Commun. (July 31, 1998).)

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Highly site-specific H_2 adsorption on vicinal Si(001) surfaces

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Abstract

Experimental and theoretical results for the dissociative adsorption of H_2 on vicinal Si(001) surfaces are presented. Using optical second-harmonic generation, sticking probabilities at the step sites are found to exceed those on the terraces by up to six orders of magnitude. Density functional theory calculations indicate the presence of direct adsorption pathways for monohydride formation but with a dramatically lowered barrier for step adsorption due to an efficient rehybridization of dangling orbitals.

(Submitted to Phys. Rev. Lett. (June 1998).)

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Positron affinity in semiconductors: theoretical and experimental studies

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Abstract

Knowledge of the positron affinity A_+, a basic bulk characteristic of materials, is important to the understanding of positron trapping at interfaces and at precipitates. Theoretical calculations of A_+ for 3C, 4H and 6H polytypes of SiC, based on various approaches to electron-positron correlations within the local density approximation and the generalised gradient approximation for positrons, are compared with experimental values obtained via work function measurements. The disagreement between theoretical and experimental values of A_+ is discussed in terms of difficulties in the precise measurement of the positron work function and the possible inadequacy of contemporary approaches to electron-positron correlation in semiconductors.

(submitted to Physical Review B)
Latex-file available from honzakr@mbox.cesnet.cz

8 Book Announcements

Relativistic Quantum Mechanics With Applications in Condensed Matter and Atomic Physics

Paul Strange

Keele University

This graduate text introduces relativistic quantum theory, emphasising its important applications in condensed matter physics. Basic theory, including special relativity, angular momentum and particles of spin zero are first reprised. The text then goes on to discuss the Dirac equation, symmetries and operators, and free particles. Physical consequences of solutions including hole theory and Klein's paradox are considered. Several model problems are solved. Important applications of quantum theory to condensed matter physics then follow. Relevant theory for the one electron atom is explored. The theory is then developed to describe the quantum mechanics of many electron systems, including Hartree-Fock and density functional methods. Scattering theory, band structures, magneto-optical effects and superconductivity are among other significant topics discussed. Many exercises and an extensive reference list are included. This clear account of relativistic quantum theory will be valuable to graduate students and researchers working in condensed matter physics and quantum physics.

Contents:

Preface; 1. The theory of special relativity; 2. Aspects of angular momentum; 3. Particles of spin zero; 4. The Dirac equation; 5. Free particles/antiparticles; 6. Symmetries and operators; 7. Separating particles from antiparticles; 8. One electron atoms; 9. Potential problems; 10. More than one electron; 11. Scattering theory; 12. Electrons and photons; 13. Superconductivity; Appendices; References; Index.

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S. Goedecker

Wavelets and their application for the solution of differential equations

Presses Polytechniques Universitaires et Romandes
Lausanne, Switzerland 1998

(ISBN 2-88074-398-2), http://ppur.epfl.ch

This book is based on a postgraduate course given by the author at EPFL in January/February 1998. The motivation for teaching this course as well as for writing this book was to make this fascinating and highly useful field of wavelets accessible to non-mathematicians. The overwhelming part of the literature on wavelets is in the classical mathematical style of theorems followed by proofs. The threshold for entering the subject for non-mathematicians is therefore rather high. In addition computational scientists, who just want to apply this theory, are more interested in an intuitive understanding of the important features instead of the formal mathematical framework. This book is intended to make the theory of wavelets understandable to this audience. In addition to a self-contained and intuitive presentation of the theory of wavelets, extensive tables with the basic filter coefficients of differential operators in several wavelet families can be found in this book. After working through this book anyone who wants to numerically solve partial differential equations in physics, chemistry or engineering using wavelets should be able to do so. Wavelets are a basis set with extraordinary properties for the solution of differential equations. Their flexibility and efficiency allows us to attack problems which are very hard or even impossible to tackle with conventional methods. It is to be expected that the theory of wavelets will soon be part of any science and engineering curriculum in the same way as Fourier analysis is nowadays.

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COMPUTATIONAL METHODS IN SOLID STATE PHYSICS

V.V. Nemoshkalenko and **V.N. Antonov**, both of *Institute of Metal Physics, Ukraine*

The combination of theoretical physics methods, numerical mathematics and computers has given rise to a new field of physics known as "computational physics." The purpose of this monograph is to present the various methods of computational physics, in particular the methods of band theory.

The first chapter of the book provides an introduction to the field and presents the theoretical foundations of band theory. In the second and third chapters the authors describe both traditional and more modern methods of band theory and include practical recommendations for their use. Methods which are discussed include APW (augmented plane wave), Green's function method, LMTO (linear method of MT- orbitals), LKKR (linear Korringer, Kohn and Rostocker method), LAPW (linear augmented plane wave), ASW (augmented spherical waves), and LASO (linear method of augmented Slater orbitals).

Great attention is paid to the practical aspects of these theories and the book is structured in such a way as to enable the reader to use any method in practice without reference to other sources.

Readership: Graduates and researchers in physics, solid state physics and band structure of solids.

October 1998, 312pp

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9 SCIENTIFIC HIGHLIGHT OF THE MONTH

Nanowires: electronic and ionic structures, cohesive and transport properties

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Abstract

The physical properties of nanowires reflect the quantum mechanical phenomena due to the confinement of the valence electron wave functions in the plane perpendicular to the wire axis. For example, the electrical conductance will be quantised. Recently, it has been realized that the characteristic electronic structure has also a direct influence on the ionic structure of the nanowire and it is not possible to separate cohesive properties and electronic properties such as conductance and capacitance.

9.1 Introduction

There is intense current interest in the physical properties of atomically-manipulated nanostructures. In such structures, quantum effects play an important rôle. Nanowires are leads where the electronic states are quantum confined to allow conduction in one dimension only. They can be produced *e.g.* by lithographic techniques on semiconductor interfaces resulting in two-dimensional electron gas systems. In this review we consider, however, three-dimensional metallic nanowires [1]. Experimentally, they can be produced in several different ways. The simplest scheme is to put two metallic protrusions in contact and then pull them from each other over atomic distances: a nanowire is produced which upon pulling is elongated and narrowed, until it eventually breaks. This basic mechanism is employed, for example, in the scanning tunneling microscopy (STM) studies of nanowires [2]. Pulling of macroscopic wires also produces nanowires. This can be done by using the sophisticated mechanically controllable break-junction technique (MCBJ) (Ref. [3]), but even simpler arrangements are sufficient [4, 5]. An interesting possibility is to produce nanowires by filling carbon or other kind of nanotubes [6]. In the experiments the conductance is usually monitored as a function of the elongation of the nanowire.

Moreover, in the atomic force microscope (AFM) experiments by Rubio, Agraït and Vieira [7] the conductance and the force during the formation and rupture of Au contacts have been measured simultaneously. A clear correlation between the force oscillations and the conductance steps during the elongation of the nanowire was seen.

Modeling of the formation of metallic nanowires in a STM experiment was first done by molecular dynamics simulations in which the atomic structure was solved using classical many-atom-type interaction potentials [8, 9]. The simulations showed that the elongation takes place through successive stress accumulation and relief stages reflecting rearrangements in the ionic structure. The calculated ionic structures were then used to determine the electric conductance by counting the available conductive channels. The scattering of the conduction electrons may be taken into account by solving for the transfer matrix for an *afterwards* constructed effective potential [10, 11, 9]. The conductance is then given by the Landauer formula [12]

$$G = G_0 \sum_i T_i(E_F), \tag{1}$$

where $G_0 = 2e^2/h$ is the conductance quantum and $T_i(E_F)$ is transmission probability for an electron entering the nanowire constriction with the Fermi energy E_F and within the channel (subband) i.

The weakness of the above procedure is that the direct correspondence between the cohesive and conduction properties through the valence electron structure is broken. The first-principles molecular dynamics simulations based on solving the self-consistent electron structures remedy this deficiency [13, 14, 15]. Indeed, this kind of simulations [13, 16] show that the atomic geometries at the neck can be derived from those of isolated small atomic clusters, the stability of which derives from the closed-shell structures of valence electrons. The rôle of the valence electron structure is emphasized in jellium-type models [17, 18, 19, 20, 21, 22], which completely ignore the detailed ionic structure. In these calculations the confinement of the valence electrons in the direction perpendicular to the wire results in an electron level structure, the subbands of which are gradually emptied as the wire elongates and its radius decreases. As a result, cohesive properties, such as the elongation force will show oscillations as the radius of the wire reduces. Moreover, because the subbands constitute the conductance channels, the conductance shows simultaneously a steplike behaviour in correlation with the force oscillations.

The electronic transport of nanowires exhibits similar quantum regimes as seen in the context of mesoscopic devices [12]. However, several new qualitative features arise. First, the length scales are comparable to the interatomic distances and therefore the atomic information cannot be summarized by a continuum model with an effective mass. Second, an essential ingredient in the scattering theory of the quantum transport is the contact to the external world. This means that the chemical interaction between the nanowire and its immediate environment is much stronger than, for instance, in the case of a tunneling contact. These issues are addressed by two complementary descriptions. Free electron models explain the conductance in terms of geometric characteristics of the wires in comparison with the Fermi wavelength [18, 23, 24]. The second class of models rationalize the experimental observations by focusing on the chemical nature of the atomic-size contacts. They decompose the conductance into contributions due to different atomic orbitals. A good example is the work by Lang *et al.* studying a wire of two

Xe atoms between leads described by the jellium model [25]. An almost quantitative agreement with experiment was found. Another example is the study of linear carbon chains showing a conductance with an even-odd dependence on the number of carbon atoms [26].

A linear chain of atoms would be the ultimate shape of a nanowire before breaking. Their existence was predicted by Sørensen *et al.* [27] by simulations based on effective-medium-theory many-atom potentials: When pulling a Au wire along the [100] direction a linear chain of six single Au atoms appeared. Recent experiments employing electron microscope imaging [28] or the measurement of the conductance as a function of elongation [29] have also shown the formation of chains which consist of several Au atoms. A puzzling results is that both experiments predict that the interatomic distance in the chain is about 3.5 ... 4.0 Å, which is considerably larger than the bond length of 2.9 Å in bulk gold. According to the effective-medium theory or first-principles calculations the equilibrium distance is smaller than the bulk distance [27].

9.2 Electronic structure and cohesive properties

In this and in the following section we review results [22] obtained by modelling the nanowires as infinitely long cylinders of stabilized jellium. Rather similar results have been obtained with a normal jellium model for wires with r_s corresponding to the valence electron density of Na [17] and with a model which considers only the kinetic energy the electrons confined by an infinite potential barrier inside the metal wire [18, 19, 20].

In the stabilized jellium model [30], the positive ionic charge is smeared to a rigid background charge with the constant density of $n_+ = 3/(4\pi r_s^3)$ within the cylinder of radius R. In contrast to the normal jellium model, a constant correction is added to the potential inside the cylinder so that the system is stable at the bulk electron density desired. The electron structure, neutralizing the positive background charge, is solved self-consistently using the local spin density (LSD) approximation. The stabilized jellium model has been shown to give a reasonable description for the surface and void energetics of simple metals [30, 31].

The eigenfunctions $\Psi_i^\sigma(\mathbf{r})$ for the infinite cylindrical geometry have the form

$$\Psi_{mnk_z}^\sigma(r,\phi,z) = \frac{e^{ik_z z}}{\sqrt{L}} \frac{e^{im\phi}}{\sqrt{2\pi}} R_{mn}^\sigma(r), \tag{2}$$

where $m = 0, \pm1, \pm2, ..$ is the azimutal quantum number, $n = 1, 2, 3, ..$ is the radial quantum number related to the number of radial nodes $(n-1)$ of the radial wave function $R_{mn}^\sigma(r)$. Further, k_z is the wave vector associated to the axial z direction along which the electrons have no restriction to move, and L is the normalization length along the z axis. Thus, the electronic structure consists of one-dimensional subbands.

The subband structure is reflected in the cohesive properties of the jellium wires as a function of the cylinder radius R. For example, the surface energy σ of the Na wires shown in Fig. 1, exhibits oscillations due to the filling of new subbands. As a result, there exist cylinder radii at which the total energy per volume has a local minimum. These (meta)stable wires correspond to the magic-number jellium spheres discussed in the context of small atomic clusters [32]. Assuming that the volume of the wire is conserved one can calculate the force needed to elongate the wire as

$$F = -\frac{dE}{dL} = -\frac{d(2\pi RL\sigma)}{dL} = -\pi R\sigma + \pi R^2 \frac{d\sigma}{dR}. \qquad (3)$$

The force is shown as a function of the radius in Fig. 2. for Na wires. Negative values mean that an external force should be applied in order to elongate (and narrow) the wire, whereas at the regions of positive force the wire would spontaneously elongate and become narrower. The prominent feature is that the force shows oscillations. The amplitude of these oscillations scales approximately as $\epsilon_F(\bar{n})/\lambda_F(\bar{n})$, where $\lambda_F(\bar{n})$ is the Fermi wavelength [18]. The magnitude of force oscillations seen in the measurements for Au is well described by this estimation [7].

The AFM experiments show stress accumulation and relief stages as the nanowire elongates [7]. The conductance is correlated with the force measured so that during the stress accumulation stage the conductivity is constant and at the relief stage it decreases rather stepwise. These notions have their counterparts in the stabilized jellium model: The step in the conductance is associated with the raise of a subband above the Fermi level. Thereafter the next subband begins to empty causing the stress accumulation while the conductance will be constant (See Fig. 1 b and c). The conductance step structure with steps of 1 G_0, 2 G_0, 2 G_0, 1 G_0 seen in Fig. 1c (for the spin-compensated case) reflects the orbital degeneracies in the cylindrical symmetry. The sequence was first predicted by Bogachek *et al.* [33] and it has been seen in the measurements for Na nanowires [3].

The next step towards a more realistic description of the actual nanowires is to consider a jellium wire with variable cross section, *i.e.* a wire with a narrow neck region [18, 34]. As a matter of fact, Yannouleas *et al.* [34] have made this step within the jellium model using their computationally efficient shell-correction method. One of their main conclusions is that the cohesive and transport properties of the wires are determined to a large extent by the electronic structure at the narrowest part of the wire. This conclusion justifies the use of model with a constant (stabilized) jellium as a first approach to the problem.

9.3 Spontaneous magnetization of simple-metal nanowires

Using the stabilized jellium model we have made the surprising finding that cylindrical wires may exhibit at certain radii spontaneous magnetic solutions [21]. They appear so that the highest energy subband is totally spin-polarized when its occupancy is small enough. The spin-polarization lowers the the surface energy and causes abrupt relief stages in the elongation force (See Fig. 1 a and b). Moreover, the conductance steps of purely spin-compensated wires are divided into two steps (Fig. 1c).

The calculations predict that at very small radii the lowest subband, which in this case is the only occupied one, will be totally spin-polarized. This kind of spontaneous spin polarization has been predicted also by Gold and Calmels [35] for cylindrical wires using the exchange-correlation energy of a quasi-one-dimensional electron gas. At first sight, the result is in contradiction with the old theorem by Lieb and Mattis [36] stating that the ground-state of a strictly one-dimensional, one-subband system should be spin-compensated. However, in our case we are dealing with three-dimensional electrons interacting via the Coulomb potential, for which the Lieb-Mattis theorem is not valid.

We can analyze the appearance of magnetic ground-state solutions of simple metal nanowires by making use of the Stoner criterion of ferromagnetism in bulk metals. The occurrence of magnetic solutions in the beginning of the occupancy of each new subband would suggest the application of Hund's rules for finite systems. But the number of electron states in a subband is not limited because a jellium wire is infinite in the z direction. From the viewpoint of an infinite system it is natural to ask whether the appearance of the magnetism in the jellium wires could resemble that in bulk metallic systems, i.e., if the Stoner criterion is applicable. According to this criterion, ferromagnetism exists whenever the condition

$$I\tilde{D}(E_F) > 1, \tag{4}$$

is fulfilled. Above, $\tilde{D}(E_F)$ is the density of states (DOS) per atom in a spin-compensated system at the Fermi level and I is the Stoner parameter for the atom in question. I is an "exchange" integral which includes also the electron-electron correlation effects.

The product $I\tilde{D}(E_F)$ is plotted in Fig. 2 as a function of the wire radius R for stabilized jellium wires corresponding to Na. For the Stoner parameter I the value for a homogeneous electron gas has been used. The peaks in the figure are due to the $1/\sqrt{E}$ divergences of the DOS at the bottoms of the subbands. The filled markers mean systems for which we have found in self-consistent electronic-structure calculations stable magnetic solutions, *i.e.* the total energy of a spin-polarized solution is lower than that of a spin-compensated one. The open markers denote then stable, spin-compensated systems. The correlation between the fulfillment of the Stoner criterion and the existence of magnetic solutions is almost quantitative. It can also be seen from the figure that the region, in which the highest subband is polarized, narrows when the radius R increases indicating the recovery of the spin-compensated bulk Na.

The appearance of magnetic solutions is a consequence of the high DOS values. In the present model high DOS values reflect the confinement perpendicular to the wire and the assumed perfect translation symmetry along the wire. For more realistic finite wire geometries we expect our prediction of magnetic solutions also to be valid in the sense that the *local* DOS at the Fermi level and at the constriction will for certain radii be so high that the Stoner criterion is fulfilled. We are not aware of direct experimental observations of the magnetic structures in the case of simple-metal nanowires. The interpretation of the conductance measurements is difficult due to the scattering probabilities $T_i(E_F)$ less than unity [23] and due to the possible orbital degeneracies. However, it is encouraging that experimental evidence of this kind for magnetic "fingerprints" exists in the conductance measurements of quantum point contacts at the interface between two different bulk semiconductors [37]. Moreover, the recent conductance results for metallic carbon nanotubes may also indicate non-trivial magnetic structures [38].

9.4 Atomic chains

The rôle of the atomic structure has not been included in the jellium calculations. We have studied the ensuing effects by calculations [39] for atomic Al and Na wires with the ab initio full potential augmented plane-wave method (FLAPW) [40]. The importance of these calculations is not only in checking the stabilized jellium predictions. They also serve as simulations for metallic atomic chains which may be realized in experiments as free-standing chains as discussed in the

Introduction or as supported ones on some insulating substrates such as silicon or an ionic material [41].

We have chosen the linear Al chain as an example because the stabilized jellium model model predicts that it should have a magnetic solution when the atomic distance is close to the nearest-neighbor bulk distance of $d_{nn} = 5.41$ au. The resulting band structure is compared with the stabilized-jellium band structure in Fig. 3. The agreement is surprisingly good supporting the use of the stabilized jellium model for Al even in the present confined geometry. The polarization of the second subband accommodating the Al $3p$ electrons is the reason for the magnetic solution. The magnetic moment per atom, 0.79 μ_b, is mainly due to this subband and it should be compared with the stabilized-jellium result of 0.69 μ_b.

We have varied the bond distance in the Al chain in order to search for the total energy minimum, as well as to study the stability of the magnetization. The results are plotted in Fig. 4. The energy minimum is found at approximately $d_{nn} = 4.5$ a.u. and it corresponds to a spin-compensated solution. The magnetization appears at distances larger than 5.1 a.u. The realization of an Al chain with such relatively large interatomic distances might be experimentally possible. Namely, for example, the normal distances of metal atoms deposited on Si surfaces are of this order [41]. Moreover, the unsupported Al chain is very soft: according to our FLAPW calculations the total energy changes only by 0.05 eV when increasing the interatomic distance by 0.2 a.u. from the equilibrium bond length. Therefore it might be possible to control the spin-polarization properties of the atomic chains by varying the structural parameters of the underlying supporting surface.

The linear chain of Na atoms with a nearest neighbor bulk distance shows no spin polarization. This is also the stabilized-jellium model prediction. Only the increase of the interatomic distance to an unrealistically large one will result in a magnetic solution. In order to demonstrate the possible existence of magnetic Na wires, we have made calculations for a planar zigzag chain of Na atoms. When the interatomic distance in this kind of chain is the nearest-neighbor bulk distance and the angle formed by three adjacent atoms is about 70 degrees, a (non-degenerate) spin-polarized p-type band appears.

Our FLAPW calculations have demonstrated that atomic chains may have magnetic solutions. However, more realistic calculations taking into account the effects due to the leads in the case of otherwise unsupported chains and the effects due to the substrate for the surface-supported chains are needed to fully explore the properties of these systems.

9.5 Quantum transport

In this section we review studies [42, 11, 43, 15, 14] which apply the scattering theory of transport [12, 45] to determine the linear transport coefficients of nanowires. The conductance and capacitance are defined as the response to a time-independent and time-dependendent external bias, respectively. The scattering potential $V_s(\mathbf{r})$ is the Kohn-Sham potential obtained by a pseudopotential-plane-wave method. The transfer-matrix technique [44] is used to solve the 3D quantum scattering problem, so that the complete scattering matrix and wavefunctions are obtained [45]. The conductance G of the wire is then evaluated as a function of the scattering energy E from the transmission part of the scattering matrix (Eq. 1). Nanowires are modeled as atomic clusters connected to two jellium leads ($r_s = 2.0$ a.u.). The clusters include diverse structures of aluminum and silicon atoms, ranging from single atoms to wires or nanoclusters.

A resonant tunneling transport regime was established for single atom contacts in Ref. [42]. The regime occurs when the contact atom is well separated from the leads so that there is a potential barrier between the atom and the both leads. The conductance is highly peaked at the scattering energy values corresponding to the atomic levels, which are now broadened, due to the atom-lead interactions, into Lorentzian resonances. When the atom-lead separation (on both sides of the contact atom) is decreased towards to the equilibrium distance the potential barriers are lowered. Thereby propagating channels are opened at the Fermi level, resulting in ballistic transport and conductance quantization.

In Ref. [11] transport properties of a linear chain of N aluminum atoms have been considered. Conductance quantizatition is seen as a function of the scattering energy E when $N \geq 2$. According to Table I the calculated resistance is systematically lower than that calculated for wires between planar electrodes [10]. The difference is due to a more abrupt contact in the latter case leading to a higher reflection of incoming electronic waves. The resistance of the atomic chains saturates for $N \geq 3$ whith the establishment of a quasi-1D behaviour. For linear chains of Si atoms a dip in the conductance at $E < E_F$ develops as N increases [43]. This reflects the energy gap between the σ and π subbands of an infinite linear Si chain.

In a microscopic conductor the discreteness of the electron density of states and the inefficient screening at distances comparable to the screening length leads to a capacitance which differs substantially from its classical counterpart. The *capacitive* response of an atomic wire is described in terms of the electrochemical capacitance $C = edQ/d\mu$ [46]. Here, dQ is the nonequilibrium charge distribution built-up in the wire due to variations $d\mu$ in the chemical potential with respect to the external reservoirs. By changing μ in the atomic junction charge is injected from the leads into the junction. The potential created by this charge induces charge polarization inside the conductor. dQ is found by solving a self-consistent Poisson equation for the characteristic potential $u(\mathbf{r}) = dV_s(\mathbf{r})/d\mu$ [46]. The screening may be approximated by a local Thomas-Fermi model.

In Ref. [14] the capacitance of different Al clusters "sandwiched" between two jellium leads has been calculated. The capacitance has been evaluated from the expression

$$C = \int_{\Omega_+} \left[\frac{dn_r(\mathbf{r})}{dE} - u(\mathbf{r}) \frac{dn(\mathbf{r})}{dE} \right] d\mathbf{r}, \tag{5}$$

where the integration volume Ω_+ is defined as the region of positive integrand values. The local density of reflected states, $dn_r(\mathbf{r})/dE$ and the total local DOS $dn(\mathbf{r})/dE$ are obtained from the scattering wavefunctions [47]. The capacitance of a five atom "tip" contact attached to one of the leads versus the distance between the leads is depicted in Fig. 5. At large distances, capacitance decreases and exhibits a geometric or classical behaviour. On the other hand, the capacitance is predicted to decrease towards to smaller distances when the separation $d < 5\mathring{A}$. This is clearly a quantum effect: the formation of the nonequilibrium charge distribution is diminished as the tunneling rate increases. The capacitance follows in this limit the reflection coefficient R of the electron waves coming from the leads, but displays more structure as seen in Fig. 6. The diverse peaked structures correspond to excitations between the reflected channel states. The excitations may even occur at the conductance plateaus. The dependence of capacitance on the atomic structure at the contact is discussed in Ref. [14]. The peak distributions provide useful information of both the structure of the contact and that of the microscopic electrodes. It is suggested that the diverse excitations could be mapped in experiments by tuning the external dc voltage or the width of the leads.

9.6 Conclusions

Atomic-scale manipulation of materials leads to a richness of nanostructures with interesting, quantum-physics-dominated phenomena. The cohesive and electronic properties of nanowires can be explored by electronic structure calculations, which reveal the atomic geometry and intricate interplay between quantised electron states and their dynamics. The electron confinement dictates the conductivity, capacitance and the elongation force of metallic wires. Simple metal wires can become spontaneously spin-polarized at suitable wire radii.

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N	channel	surface(Ref. [10])
1	4.7 (2.5)	6.6 (2.0)
2	7.9 (1.6)	9.0 (1.4)
3	5.1 (2.5)	8.3 (1.6)
4	5.3 (2.4)	–

Table 3: Resistance (in KΩ) of a linear chain of Al atoms versus the chain length, N. In the parentheses, the conductance in units of of $G_0 = 2e^2/h$.

Figure Captions

Fig. 1. Surface energy (a), elongation force (b) and conductance for Na stabilized-jellium wires as a function of the wire radius (solid lines). In (a) the results of the extended liquid-drop model are also given by a dashed line [31]. When the wire radius increases the surface energy approaches that [31] for a planar stabilized-jellium surface. In (b) the forces derived from the surface energy of a planar surface ($-\pi R\sigma_{planar}$) are shown by a dashed line. The conductance in (c) is obtained from Eq. 1 by assuming $T_i(E_F) \equiv 1$. In (a) and (b) values corresponding to spin-polarized solutions are shown as black circles. In (c) unstable spin-compensated solutions are given with dashed lines.

Fig. 2. Stoner criterion product $I\tilde{D}$ for Na stabilized-jellium wires as a function of the wire radius. The regions of stable magnetic and spin-compensated solutions are denoted by filled and open markers, respectively.

Fig. 3. Band structure of a linear chain of Al atoms. The interatomic distance is the nearest-neighbor bulk distance of $d_{nn} = 5.41$ au. Majority and minority-spin bands calculated by the FLAPW method are shown by filled and open circles, respectively. They are compared with the corresponding stabilized-jellium-model results given solid and dashed lines.

Fig. 4. Total energy (a) and the magnetic moment per atom for a linear chain of Al atoms as a function of the interatomic distance. The results calculated by the FLAPW method for the spin-compensated and for the spin-polarized system are given by dashed and solid lines, respectively.

Fig. 5. The electrochemical capacitance C for the 5-atom tip-substrate system as a function of the distance d between the tip and the substrate: (a) classical and (b) quantum calculations. Details of the structure can be found in Ref. [14].

Fig. 6. Capacitances of the 5-atom tip junction. These systems are characterized by resonance transmission. Solid lines: $C(E)$ in units of 0.01aF. Dotted lines: $G(E)$ in units of $2e^2/h$. Dashed lines: the total reflection probability R.

Figures

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