HCM Newsletter

Ψ_k Network

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

Number 22 August 1997

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Contents

1 Editorial

In this *Newsletter* we have a report on the Bogoliubov de Gennes Workshop which contains abstracts of most contributed papers. In the **Highlight of the Month** section of the Newsletter readers will find two short articles. The first one is by Volker Heine (*Cambridge*) and Björn Winkler (*Kiele*) on *'Applying Ab Initio Calculations in Mineralogy'*, and the second one features a very fruitful collaboration of the present Network between the groups of Mike Gillan (*Keele*) and Jürgen Hafner (*Vienna*).

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

The above contains pointers to several other nodes: *O.K. Andersen (Stuttgart)*, *P. Blöchl (IBM, Zürich)*, *M. Finnis (Univ. Belfast)*, *M. Gillan (Univ. Keele)*, *E.K.U. Gross (Univ. Würzburg)*, *B.L. Györffy (Univ. Bristol)*, *M. Heggie (Univ. Sussex)*, *V. Heine (Univ. Cambridge)*, *R. Jones (Univ. Exeter)*, *J. Kübler (TH, Darmstadt)*, *R. Nieminen (TU, Helsinki)*, *J. Nørskov (TU, Lyngby)* with information on CAMP, *M. Scheffler (FHI Berlin)*, *K.-H. Schwarz (TU, Vienna)*, *M. Springborg (University of Konstanz)*, *G.P. Srivastava (Univ. Exeter)*, *W.M. Temmerman (Daresbury Laboratory, UK)*, and *A. Walker (UEA Norwich)*. There also exists a pointer to the WWW home page of the Solid State Theory Group at National Renewable Energy Laboratory, Golden, CO 80401 *(http://www.sst.nrel.gov)*. If you maintain a home page on your activities we will be happy to include a pointer from the *Network's* home page to your home page.

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

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

	function
psik-coord@daresbury.ac.uk	**messages to the coordinator & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB**
psik-network@daresbury.ac.uk	**messages to the whole Network**

Dzidka Szotek & Walter Temmerman
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2 News from the Network

The good news is that our proposal for a TMR Research Network on '**Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Sciences**', which was submitted to the EU Commission at the end of January, as a successor to the Ψ_k-Network, has been successful. We are in the process of negotiating the final contract with the EU Commission. TMR Networks are much more research and project orientated than HCM Networks, but we incorporated in the proposal for the TMR Network a node dedicated to training and dissemination to keep many of the present HCM Ψ_k- Network activities going. Moreover, after signing the final contract, the new Network will have eight three year postdoctoral positions available to work on the main projects of the proposal. For details on the projects readers are advised to see the section **New TMR Network** in this Newsletter. The postdoctoral positions, for which only EU nationals are eligible, will be advertised in detail in one of the future newsletters.

Concerning our ESF application for a five year programme, it has been strongly recommended by the ESF Secretariat for funding by all member countries participating to the ESF. Both the funding and final details need to be negotiated, but we are very hopeful for the best. If fully successful, also scientists from the countries of Central Europe will be able to benefit from the programme. Moreover the funding will be mostly for the kind of activities that have underlined the present HCM Ψ_k-Network.

3 News from the Working Groups

3.1 Reports on Collaborative Visits

Report on a Collaborative Visit of M. W. Finnis (Belfast) to Max-Planck Institutes in Stuttgart

May 20-25, 1997

The purpose of this visit was to continue two collaborations.

At the Institute für Festkörperforschung I had discussions with Volker Heine and Carla Molteni on the mechanisms of grain boundary sliding and other kinds of deformation in aluminium. With Dr. Molteni I helped construct a unit cell in which the interaction of a dislocation with a twin boundary could be studied. The plan is to study the atomic configurations at the atomic core as it enters the grain boundary under the influence of an applied shear, first with semi-empirical potentials and then *ab initio*.

At the Institut für Metallforschung I discussed calculations on metal-oxide adhesion with Sybille Koestlmeier and Christian Elsässer, who are studying the surface of spinel interacting with Ag and Al, using a mixed-basis pseudopotential code. There is parallel experimental work led by Frank Ernst, which is giving information about the location of the Al atoms at the surface. These are the people I would be collaborating with in any extension to the present project. I also worked on a paper on *ab initio* calculations of a grain boundary in alumina, the structure of which Martin Exner has been steering to convergence using CASTEP. Further work is needed to compare the *ab initio* structure with the structure predicted by semi-empirical potentials.

Mike Finnis

Report on a Collaborative Visit of B.L. Gyorffy (Bristol) to Max-Planck Institute in Stuttgart

July 9-10, 1997

I visited Ole Andersen at the Max-Planck-Institute in Stuttgart on July 9 and 10. We had a long and fruitful discussion during which we resolved all our differences concerning the text of our forthcoming paper on the quasi-paricle spectra of high temperature superconductors. We also had the opportunity to plan ahead and we decided to continue our collaboration on this topic focusing on the doping dependence of the transition temperature T_c during the next few months. It was a fruitful and pleasent visit.

Balazs L. Gyorffy

Report on

Third HCM - W O R K S H O P

Full-Potential LAPW Calculations with the new WIEN97 Code

Vienna University of Technology, Vienna, Austria

July 2-5, 1997

Chairman: K. Schwarz (TU Wien)

Sponsors:

Human Capital and Mobility Programme

Creditanstalt Bankverein

TU Wien and its Computing Center

This third workshop was concerned with recent progress in density functional calculations using the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the new WIEN97 code. The workshop had a dual purpose, the presentation of the new WIEN97 program package and the presentation and discussion of various scientific results obtained with the FP-LAPW or related methods. The HCM workshop lasted for four days and was attended by 64 researchers from fifteen countries. The scientific programme covered a short introduction (by K. Schwarz) to Density Functional Theory (DFT), band structure methods in general and the LAPW method, with corresponding algorithms and features, in particular. The outline and the handling of the program package was described in detail by P. Blaha assisted by J. Luitz, who illustrated the new graphical user interface by performing the corresponding calculations life for the simple test cases discussed. In addition to this demonstration the participants had plenty of time to run WIEN97 on several workstations in five excercise sessions. This arrangement was well accepted by all (experienced and novice) users, who could perform "hands-on" calculations with the user-friendly code and learned by practice. This part was supplemented by lectures on new features of the code, namely the spin-orbit coupling (by P. Novak), the efficient solution of the general eigenvalue problem (by D. Kvasnicka) and the calculation of optical properties (by Claudia Ambrosch).

In the second part applications directly or indirectly related to the WIEN95/WIEN97 package were presented as lectures or posters illustrating many interesting band structure results such as relative phase stability, phase transitions, spin-orbit splitting, electric field gradients, Fermi surfaces, photoemission or x-ray emission and absorption spectra. The solids that were investigated ranged from semiconductors, intercalation compounds, surfaces, intermetallics to minerals. In addition to these topics computational aspects were discussed, e.g. fine grain parallelization of the code (a coarse grain version on the k-point level is already available).

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

The full list of participants is included below:

Robert Abt (*KFA Juelich, Germany*)
Philipp, A. Aebi (*Fribourg, Switzerland*)
Elena Akhmatskayai (*Uxbridge, UK*)
Roberto E.Alsono (*La Plata, Argentina*)
Claudia Ambrosch-Draxl (*Graz, Austria*)
Andres Ayuela (*Espoo, Finland*)
Mario Bandic (*Fritz-Haber Institut, Berlin, Germany*)
Lean-Luc Barras (*Fribourg, Switzerland*)
Peter Blaha (*TU Vienna, Austria*)
Gianluigi Botton (*Cambridge, UK*)
Marc Bovet (*Fribourg, Switzerland*)
Ching-Ming Wei (*Taipei, Taiwan*)
Stefaan Cottenier (*KU Leuven, Belgium*)
Joerg Dewitz (*TU Berlin, Germany*)
Pavol Dudesek (*TU Berlin, Germany*)
Hartmut Enkisch (*Dortmund, Germany*)
Gabriel Fabricius (*La Plata, Argentina*)
Gilles Frapper (*Ottawa, Canada*)
David Garcia (*Madrid, Spain*)
Regis Gautier (*Rennes, France*)
Jacek Goniakowski (*Marseille, France*)
Mikko Hakala (*Helsinki, Finland*)
Michael Hartung (*Siegen, Germany*)
Jens Hattendort (*Fritz-Haber Institut, Berlin, Germany*)
Sylvia Hellwig (*Dortmund, Germany*)
James Hess (*Lehigh Univ., PA, USA*)
Carsten Holtfort (*Duisburg, Germany*)
Serguei Khmelevski (*Praha, Czech Republic*)
Kamil Klier (*Lehigh Univ., PA, USA*)
Jost Koller (*TU Clausthal, Germany*)
Robert Kouba (*Graz, Austria*)
Dieter Kvasnicka (*TU Vienna, Austria*)
Knut Lie (*Trondheim, Norway*)
Ana Maria Llois (*Buenos Aires, Argentina*)
Joachim Luitz (*TU Vienna, Austria*)
Franisek Maca (*Praha, Czech Republic*)

Maria del Carmen Michelini (*La Plata, Argentina*)
Peter Mohn (*TU Vienna, Austria*)
Michael Nelhiebel (*TU Vienna, Austria*)
Pavel Novak (*Praha, Czech Republic*)
Marek Olsovec (*Praha, Czech Republic*)
Krzysztof Osuch (*TU Clausthal, Germany*)
Anton Paintner (*Munich, Germany*)
David Pankhurst (*Cambridge, UK*)
P. Ravindran (*Uppsala, Sweden*)
Osvaldo Rodriguez (*La Plata, Argentina*)
Andres Saul (*Marseille, France*)
Samir Sawaya (*Marseille, France*)
Lothar Schimmele (*MPI Stuttgart, Germany*)
Walter Schirmacher (*TU-Munich, Germany*)
Karlheinz Schwarz (*TU Vienna, Austria*)
Bruno Siberchicot (*CEA, Villeneuve St. George, France*)
Mark Sifkovits (*Dortmund, Germany*)
Antonin Simunek (*Praha, Czech Republic*)
Elisabeth Sjosted (*Uppsala, Sweden*)
Holger Smolinski (*Dortmund, Germany*)
Mojmir Sob (*Brno, Czech Republic*)
Jorge Osvaldo Sofo (*Bariloce, Argentina*)
Pascal Thibaudeau (*Monts, France*)
Andrij Tymoshevskyy (*Kiev, Ukraine*)
Peter Vansant (*Antwerpen, Belgium*)
Ligen Wang (*Brno, Czech Republic*)
Bernd Zangger (*Graz, Austria*)
Bernd Zellermann (*Munich, Germany*)

(Karlheinz Schwarz)

Report on

The IVth International Workshop on Solving the Bogoliubov-de Gennes Equations for Superconductors

Sponsored by: CCP9 and EU–HCM ψ_k-Network

Organized by: **B.L. Györffy** (blg@siva.bris.ac.uk)
W.H. Beere (bill.beere@bris.ac.uk)
W.M. Temmerman (W.M.Temmerman@dl.ac.uk)
Burwalls, Bristol, July 12-13, 1997

The workshop was held at Burwalls, a conference center belonging to the University of Bristol, on the weekend of the 12th-13th July. It was organized by W.H. Beere and B.L.Györffy and was sponsored by the Computational Collaborative Project 9 (CCP9) of the UK and the European Human Capital and Mobility (EU-HCM) Psik-Network.

As the enclosed Program and abstracts indicate, once again, we covered those areas of superconductivity where numerical solution of the Bogoliubov-de Gennes (BdG) equations play a significant role. For the first time we have discussed the quasi-particle spectra of the high-temperature superconductors both in the normal (Dasgupta) and the superconducting (Szotek) states on roughly equal footing (LMTO 8-band model). Another novelty was a careful discussion of the photoemission experiments (Beere and Kaye) which purport to measure the Fermi-surface in the normal state and the k-dependence of the gap in the superconducting state (we were not fully convinced). The Recursion Method was again shown to be a powerful method for solving the BdG equations on a lattice with complex geometry like a grain boundry (Martin). Both formal theory (Gross, Capelle and Lüders) and applications (Seviour, Leadbeater and Sweeney) were reporting new results. We also heared a very useful summary of the current state of play concerning the High-T_c saga as was perceived by the key players at the Varenna meeting a week earlier (Alexandrov).

It was a scientifically interesting and truely pleasant occasion.

(Bill Beere & Balazs Györffy)

List of participants

Rob Seviour	Lancaster	seviour@unix.lancs.ac.uk
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Programme:

Saturday 12^{th} July

11.00 - 1.00	*Chairman*	Balazs Györffy
11.00 - 11.40	I. Dasgupta (*Stuttgart*)	**Low Energy Hamiltonians for High T_c Superconductors**
11.40 - 12.20	Dzidka Szotek (*Daresbury*)	**Quasi-particle Spectra of High Temperature Superconductors**
12.20 - 1.00	Hardy Gross (*Würzburg*)	**Magnetooptics and new density functionals for superconductors**
2.00 - 4.00	*Chairman*	Walter Temmerman
2.00 - 2.40	Kevin Duncan (*Bristol*)	**de Haas-van Alphen Oscillations in the Superconducting State**
2.40 - 3.20	Andrew Martin (*Bristol*)	**Interfaces of s- and d-wave Superconductors**
3.20 - 4.00	A.S. Alexandrov (*Loughborough*)	**Evidence for the Charged Bose Gas in the Cuprates**
4.30 - 6.30	*Chairman*	James Annett
4.30 - 5.00	Vincent Sweeney (*Lancaster*)	**Effective transport in superconducting/ferro nano-structures**
5.00 - 5.20	Terro Heikkila (*Lancaster*)	**Thermal properties of d-wave supercondtivity**
5.20 - 5.50	Robert Seviour (*Lancaster*)	**Conductance suppression in the n-s hybrids**
5.50 - 6.30	Mark Leadbeater (*Dresden*)	**Phase-Periodic Transport in N-S Structures**

Sunday 13^{th} **July**

9.00 - 10.20	*Chairman*	O. Jepsen
9.00 - 9.40	George Kaye (*Cambridge*)	**Angle Resolved Photoemission from the Cuprates**
9.40 - 10.20	Bill Beere (*Bristol*)	**Photoemission from the High T_c Superconductors**
10.50 - 12.50	*Chairman*	A.S. Alexandrov
10.50 - 11.30	Jonathan Wallington (*Bristol*)	**Unified approach to magnetism and superconductivity**
11.30 - 12.10	Klaus Capelle (*Würzburg*)	**Group-theoretical analysis of relativistic order parameters**
12.10 - 12.50	Martin Lüders (*Würzburg*)	**The exact Kohn-Sham gap equation**

Low Energy Hamiltonians for High T_c Superconductors

I. Dasgupta , O. Jepsen, and O. K. Andersen

Max-Planck-Institut Für Festkörperforschung, Stuttgart, Germany

Abstract

The recently developed TB-LMTO-ASA downfolding technique is employed to obtain orthogonal, two-centered, nearest-neighbor tight-binding model Hamiltonians for the CuO planes for several High T_c cuprates. We show that our model is generic and is capable of reproducing the non-trivial details of the low energy LDA band structure, in particularly those arising from the dimpling of the CuO planes and variation of the apical oxygen distance to plane Cu. We use this model to compute the electron-phonon interaction for the buckling mode with dimpled CuO planes and show it can support d-wave-gap-anisotropy.

Quasi-Particle Spectra of High Temperature Superconductors

B.L. Gyorffy[a], Z. Szotek[b], W.M. Temmerman[b],
O.K. Andersen[c] and O. Jepsen[c]

[a] *H H Wills Physics Laboratory, University of Bristol, UK*

[b] *Daresbury Laboratory, Warrington, UK*

[c] *Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany*

Abstract

We present a semi-phenomenological approach to calculating the quasi-particle spectra of High Temperature Superconductors. It is based on a particularly efficient parametrisation of the effective electron-electron interaction afforded by the Density Functional Theory for superconductors and a Tight-Binding-Linearized-Muffin-Tin-Orbital (TB-LMTO) 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 details. We compare our results for the gap function $\Delta(\mathbf{k})$ on the Fermi Surface with those deduced from photoemission experiments on single crystals of $YBa_2Cu_3O_7$ (YBCO). We also compare our predictions for the temperature dependence of the specific heat with measurements 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. Preliminary results on the dependence of T_c on doping for this interaction and the on-site $d_{x^2-y^2}-d_{x^2-y^2}$ paring interaction are also presented.

Density functional theory of the superconducting state: Towards new xc functionals

E.K.U. Gross, S. Kurth, M. Lüders and M. Marques

Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D - 97074 Würzburg, Germany

Abstract

Density functional theory provides a rigorous description of superconductors in thermal equilibrium in terms of the density and the superconducting order parameter. These two "densities" are determined by a set of Kohn-Sham-type equations describing the superconducting state. These equations are structurally similar to the traditional (mean-field) Bogoliubov - de Gennes equations but, in contrast to the latter, incorporate both normal and superconducting exchange-correlation (xc) effects. Neglecting the vertical coupling between different bands, these density-functional Bogoliubov - de Gennes equations can be decoupled into a normal Kohn-Sham equation and a gap equation which have to be solved self-consistently with each other. The gap equation contains, in addition to the usual BCS term, an xc pairing potential. LDA-type approximations for the latter are derived on the basis of many-body perturbation theory. To this end an RPA resummation of all normal and anomalous bubble diagrams is performed for the homogeneous electron gas. Finally it is outlined how the effective particle-particle interaction and hence the superconducting mechanism can be identified, once an approximation for the (universal) xc functional is given.

de Haas-van Alphen Oscillations in the Superconducting State

K.P. Duncan and B.L. Györffy

Bristol University

Abstract

We generalise the semi-classical theory of electrons in a magnetic filed to deal with the case of superconductors. In particular we discuss the quasi-particle spectrum of the Abrikosov flux lattice and present calculations fo the local DOS at verious r points in the unit cell of the flux lattice. The method of Weyl quantisation is then used to investigate the superconduting analogue of Landau levels and describe the machanism of de Hass-van Alphen oscillations in the superconducting state.

Properties of d and s wave interfaces.

A.M. Martin, J.F. Annett

H.H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, Bristol BS8 1TL, United Kingdom.

Abstract

We will demonstrate how to solve the Bogoliubov de Gennes equation, in a self-consistent manner, using the recursion method, where the interaction of interest can either be local or non-local. The system we shall consider will be a tight binding lattice with nearest neighbour hopping and interactions which can either be on-site or nearest neighbour. This will allow us to study both systems where the interactions remain constant throughout the system and situations where the interaction can change from site to site. Having presented the method for solving the Bogoliubov de Gennes equation we will then proceed to consider some specific examples. The first of these will be systems where the interaction remains constant throughout the system, the solutions for this system when the interaction is local will be a local s-wave order parameter. Then we will consider a non-local interaction and find two possible solutions extended s and d-wave, we will note that for the systems we are concerned with that the d-wave solution is more stable. Having considered systems where the interaction is uniform throughout the lattice we will proceed to look at systems where the interaction changes in a step like manner between two regions. We will present results for calculations of the local particle density of states as one moves across different interfaces. The three interfaces of interest will be a normal s-wave interface, a normal d-wave interface and an s-wave d-wave interface. From the calculations presented for these interfaces it will be seen that the local particle density of states has a rich structure which is not present when one performs a non-self-consistent calculation.

2e Charge Bose-liquid in High Tc Superconductors

A. S. ALEXANDROV

Department of Physics, Loughborough University, Loughborough LE11 3TU, UK.

Abstract

There now exists strong experimental evidence that the superconducting carriers in cuprates and doped fullerenes are small polarons and bipolarons [1]. We show by the use of the generic Hamiltonian including the electron-phonon interaction and the direct Coulomb repulsion that the ground state of doped Mott insulators is a charged 2e Bose liquid of small bipolarons if the electron-phonon coupling constant l is of order or larger than unity [2]. Hole bipolaron band structure is derived for perovskites. The high value of superconducting Tc, its "boomerang" doping dependence as well as the divergent upper critical field and l-like specific heat in cuprates are described. A microscopic theory of the normal state in-plane and c-axis transport of copper oxides is developed. The temperature and doping dependence of the in-plane and out-of-plane resistivity as well as the spin susceptibility are found in a remarkable agreement with the experimental data in underdoped, optimally and overdoped cuprates for the entire temperature regime from Tc up to 600 K. The normal state gap is

explained and its doping and temperature dependence is clarified. [1] K. A. Muller, Plenary talk at M2HTSC-V (Beijing, March 1997). [2] A.S. Alexandrov and N.F. Mott, "High Temperature Superconductors and Other Superfluids", Taylor & Francis (1995); "Polarons and Bipolarons" World Scientific (1996).

Electronic Transport In Superconducting - Ferromagnetic Nanostructures

V.Sweeney, C.J.Lambert

School of Physics and Chemistry, Lancaster University LA1 4YB, Lancaster UK

Abstract

We derive a spin dependant Bogoliubov-de-Gennes equation and use it to study how the presence of a magnetic moment affects the transport properties of mesoscopic systems in the change from a NS (normal - superconductor) structure to that of the FS (ferromagnetic - superconductor).

The main point of interest is that of the Zero Bias Anomaly [1] (a N-I-S system) and show how an incresing magnetic moment in the disordered normal region shifts the ZBA peak to finite energies and also how it modifies the magnitude of the effect.

Phase-Periodic Transport in N-S Structures.

M. Leadbeater

Max-Planck-Institut fur Physik, Komplexer Systeme, Bayreuther Str. 40-Haus 16, 01187 Dresden, Germany.

Abstract

We solve the Bogoliubov de Gennes equation to calculate transport properrties of mesoscopic normal/superconducting hybrid structures. The emphasis of this talk will be to discuss specific transport phenomina which occur in the mesoscopic limit. For example the conductance of different N-S interfaces will be discussed and such properties as zero-bias anomally will be highlighted. We will then move on to discuss recent experiments in phase peridic transport. We will show how in simple cases the conductance of a mesoscopic system can be modulated by phase differences between different superconducting regions. We will then proceed to consider specific experimental results and compare these with theoretical predictions, which have been made by solving the Bogoiubov de Gennes equation. Specific examples will include how the conductance of a mesoscopic normal cross, with two superconductors attached to the ends of two of the branches, is modulated by the phase difference between the two superconducting regions and how the conductance of an N-S structure is modified if there is a supercurrent in the superconducting region travelling perpindicular to the N-S interface. Finally we will conclude by highlighting different results between calculations performed by solving the Bogoliubov de Gennes equation and approximations to this equation, for example the Elinberger equations.

[1] A. Kastalsky, A.W.Kleinsasser, L.H.Greene, F.P.Milliken, and J.P.Harbison, Phys. Rev. Lett. **67**, 3026 (1991).

Interpretation of the ARPES normal state gap in cuprate superconductors from a mixed boson-fermion model

G.J. Kaye

IRC in Superconductivity, Cambridge University

Abstract

Recent ARPES measurements have revealed a loss of spectral weight in the incoherent signal at the Fermi surface crossing whose magnitude seems to have the '$d-$wave' symmetry of the superconducting gap. In this paper we present a calculation of the signal expected from a mixed state of polarons and bipolarons and demonstrate that the feature can be interpreted as a signature of the internal symmetry of the bipolarons rather that of a true 'gap'. We also postulate that the pseudogap is an intrinsic feature of the *incoherent* background contrasting with the superconducting gap, thought of as a gap in the *coherent* signal, the latter being unresolvable in the underdoped materials.

Photoemission from the High T_c Superconductors

W.H. Beere & J.F. Annett

Bristol University

Abstract

We discuss the use of the fluctuation exchange(FLEX) approximation, as described by Scalapino et.al. Using this approximation we investigate the one band Hubbard model with positive on-site interaction. Obtaining the spectral functions and the density of states we find some interesting features form this simple model. We observe the pinning of the peak in the density of states to the Fermi-surface. The width of the spectral function at the Fermi-surface is also observed to be a function of position on the Fermi-surface, which qualitatively agrees with the ARPES data from many of the high T_c superconductors. We also observe enhanced scattering around the van-Hove singularity, where at half filling the scatteing increases towards the Fermi-surface at the van-Hove singularity.

A Unified Approach to Superconductivity and Magnetism.

Jonathan P. Wallington & James F. Annett

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University of Bristol,
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United Kingdom.

Abstract

The Hubbard model, at half-filling, has two continuous $SU(2)$ symmetries - spin and 'pseudospin' (charge/pairing). In addition, charge conjugation, time reversal and the Lieb-Matthis transformation $\left[c_\uparrow(r) \mapsto c_\uparrow(r), c_\downarrow(r) \mapsto (-1)^r c_\downarrow^\dagger(r)\right]$ which interchanges spin and pseudospin, form a discrete symmetry group.

We calculate the representations of this group of discrete symmetries and use them to factorise the Hubbard interaction Hamiltonian in such a way that all the symmetries are explicit. Adopting a four-spinor notation allows us to deal with both spin and pseudospin on an equal footing and to examine the the effects of one on the other via the use of the Hubbard-Stratonovich transformation. Results for mean field theory are presented and an effective Landau-Ginzburg-Wilson functional, incorporating interacting spin and pseudospin, is introduced.

Group-theoretical analysis of relativistic order parameters

Klaus Capelle and E.K.U. Gross

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Abstract

The requirement that every fundamental theory of nature must be Lorentz invariant leads to constraints on the possible superconducting order parameters. By an analysis of the irreducible representations of the Lorentz group it is found that relativity allows five distinct types of order parameters with a total of sixteen components. This finding is contrasted with the nonrelativistic result that there are only two types of order parameters (namely those for singlet and triplet superconductivity) with a total of four components.

We prove that there can be no further types of order parameters than these five. For each of them we work out the transformation behaviour, an explicit representation in terms of Dirac matrices, the relation to the discrete symmetries of the Dirac equation and the nonrelativistic limit. In this limit one recovers the BCS and Balian-Werthamer order parameters for singlet and triplet superconductors, respectively. Going beyond this limit we find relativistic corrections to the conventional theory of superconductivity as well as new forms of superconductivity which are not present in a completely nonrelativistic theory.

It is pointed out that these findings are of relevance for a number of observable quantities, in particular for superconductors containing heavy elements, such as the heavy-fermion compounds or the high-temperature superconductors.

The exact linearized Kohn-Sham gap equation

Martin Lüders and E. K. U. Gross

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Abstract

It has been shown that the density functional theory for the superconducting state can be *approximately* reformulated in terms of a normal Kohn-Sham Schrödinger equation, and a gap equation, which, in contrast to the BCS gap equation contains exchange and correlation terms. In this way the energy scale of the electronic bandstructure and the energy scale of the superconducting gap can be decoupled. Here we show that in the vicinity of the transition temperature an *exact* decoupling can be achieved, leading to an *exact* generalization of the Kohn-Sham gap equation. This is shown by employing the thermodynamic argument that the normal state gets unstable with respect to an infinitesimal perturbation below T_c. The phase transition is thus characterized by a divergence of the linear response function, or equivalently a vanishing inverse response function. This linear response function is calculated exactly in the Kohn-Sham system, and the condition for a zero eigenvalue of the inverse response function yields the linearized gap equation. It is also shown that this equation contains the gap equation of the decoupling scheme and the BCS gap equation as special cases.

Report on

Symposium D - 1997 ICAM and E-MRS Spring Meeting: Computational Modeling of Issues in Materials Science.

Partially supported by the HCM network
"Ab-initio calculation of complex processes in materials".

Strasbourg (France), June 16 - 20, 1997

With 181 submitted abstracts and 12 sessions running for the entire duration of the meeting, this was the largest symposium at the conference. Attendants came from all five continents, with participants from as far away as South Africa and Australia. Also a large representation from Eastern Europe was present.

The symposium was kicked off with a plenary talk by Prof. Volker Heine (Cambridge University) entitled: 'The design of "computer experiments"'. This speaker emphasized the predictive power of computer calculations, the possibility of accessing regions in parameter space that cannot be attained by experiment, and the ability of simulations to provide virtually unlimited space and time resolution. He also stressed the need for computer experiments to provide 'understanding', which allows a massive amount of data to be collapsed in a few simple rules.

The remainder of the symposium consisted of a series of lively sessions with the following titles: 1. General simulation methods; 2. Ab initio and tight-binding molecular dynamics; 3. Surfaces and films; 4. Complex materials and parallel computing; 5. Fracture; 6. Polymers; 7. Micromagnetism; 8. Magnetism; 9. Electronic structure (specific materials); 10. Electronic structure (methodology); 11. Complex materials and alloys; and 12. Clusters. There were 14 invited talks, 54 contributed papers, and 62 posters (divided over two sessions) actually presented at the symposium.

It became evident at the meeting that computational materials science has truly emerged as a field in itself. The range of phenomena studied and the variety of techniques used were truly astonishing and indicate that the subject has sufficiently matured that technologically relevant information can now routinely be extracted from computational modeling. Moreover, these models increasingly use atomistic information (frequently in the form of 'ab initio' calculations) from which macroscopic parameters may be determined.

The contributions and discussions at this symposium clearly indicated that some major themes have emerged. Several papers showed that parallel computers will play a major role in the further development of the field: simulations with 100 million atoms, approaching macroscopic

dimensions, have now become possible on the latest parallel hardware. Clearly, new algorithmic ideas will be needed and, in particular, scalable software will be essential for further progress. Thus, so-called order-N methods were the subject of lively debate.

Another clear trend was the emergence of the Car-Parinnello method as a workhorse for the most advanced simulations, simultaneously combining electronic structure and molecular dynamics optimization. Only a few years ago it was considered computationally very expensive and of such a sophistication that only experts could use it. The advent of faster hardware and the diffusion of computer codes have brought this technique within the reach of many research groups.

The local density approximation (LDA) of the density functional theory (DFT) has been at the center of much work in electronic structure calculations for several decades. Although it has been remarkably successful, a number of its limitations have been known for a while and several authors at the meeting discussed schemes for going beyond LDA.

Atomistic simulations frequently operate on microscopic time and length scales: nanometers and femtoseconds are the basic units in this realm. The macroscopic world however operates on a very different scale. While a correct description of many observations requires quantum mechanics for a true understanding, the relevant measurements are done on the macro-scale. How to consistently go from the micro- to the macro-scale (and also describe the intermediate meso-scale) remains one of the great unsolved puzzles in computational materials science and was the subject of much discussion at the symposium.

Science often progresses by analogies: techniques that are valuable in one field are frequently found to be also applicable in another. The interdisciplinary side of computational studies of matter was demonstrated in several talks, where authors borrowed methods from nuclear physics, fluid dynamics, and other subjects.

The organizers benefited greatly from the expert advice provided by the members of the International Organizing Committee. They include: V. Alessandrini (Paris, France), K. Binder (Mainz, Germany), J. Connolly (Lexington, USA), P.H. Dederichs (Jülich, Germany), M. Doyama (Tokyo, Japan), R.A. de Groot (Nijmegen, The Netherlands), J. Hafner (Wien, Austria), V. Kumar (Kalpakkam, India), A.A. Lucas (Namur, Belgium), J.L. Moran Lopez (San Luis Potosi, Mexico) and A. Zangwill (Atlanta, USA).

Financial assistance for the symposium was provided by the Université Louis Pasteur (Strasbourg), the Institut de Physique et Chimie des Matériaux de Strasbourg, the Ministère de l'Enseignement Supérieur et de la Recherche for supporting travel and lodging expenses of Eastern European participants and by the European HCM network Ψ_k " Ab initio (from electronic structure) calculation of complex processes in materials". The support from these organizations was essential and is gratefully acknowledged.

All in all, this was a very productive symposium. New collaborations were started, many novel ideas were generated, and a large amount of information was disseminated. Because of the wide range of subjects, participants gained new appreciations for the scope of the field but also for the unity that has emerged. The meeting gave an excellent idea of the status of computational materials science anno 1997. It is hoped that the reader will find in the proceedings which will

appear in a special issue of Computationanl Materials Science, a more permanent record of these developments.

CHAIRPERSONS

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4 Conference Announcements

4.1 CECAM Workshop on Reactivity at Surfaces

Final Announcement

Lyon, 28-30 August 1997
Organizers: **A. Selloni and M. Scheffler**

The workshop will consist of a series of invited talks and a poster session. A detailed (tentative) program can be found at the WEB site: http://sc2a.unige.ch/ selloni/cecam.html

Registration can be sent to A. Selloni (email: selloni@sc2a.unige.ch) or M. Scheffler (email: scheffler@fhi-berlin.mpg.de).

There is no registration fee.

Motivation and objectives:

The objective of this workshop is to bring together scientists with different backgrounds (chemistry, condensed matter physics, materials science, computational physics, etc.) in order to discuss current issues and perspectives in the theoretical modeling of chemisorption and reaction of adsorbates on metal and insulator (e.g. semiconductor and oxide) surfaces.

Topics of interest include:

- First principles electronic structure calculations. Accuracy of various gradient-corrected functionals in the evaluation of reaction profiles.
- Models used to represent the surface: clusters vs slabs; embedding methods.
- Methods for finding saddle points on the potential energy surface.
- Dynamical effects. Analysis of the importance of the high dimensionality of configuration space. Quantum mechanical effects in the motion of the nuclei.
- Systems of very large size: semi-empirical methods; O(N) techniques.
- Calculations of electronic spectra: status and perspectives.

List of speakers:

E.J. Baerends - *VU, Amsterdam, NL*
D.M. Bird - *University of Bath, UK*
P. Blöchl - *IBM-Zurich, CH*

F. Buda - *SNS, Pisa, Italy*
E.A. Carter - *UCLA, USA*
R. Del Sole - *Universita di Roma II, Italy*
A. De Vita - *IRRMA, Lausanne, CH*
M. Gillan - *University of Keele, UK*
A. Goursot - *NSC, Montpellier, France*
A. Gross - *FHI, Berlin, Germany*
S. Holloway - *University of Liverpool, UK*
K. Jordan - *University of Pittsburgh, USA*
P. Kratzer - *FHI, Berlin, Germany*
G. Pacchioni - *University of Milano, Italy*
M.C. Payne - *Cavendish Laboratory, UK*
L.G.M. Pettersson - *Stockholm, Sweden*
D.R. Salahub - *University of Montreal, Canada*
K. Stokbro - *DTU, Lyngby, Denmark*
V. Termath - *Humboldt, Berlin, Germany*
V. Stämmler - *Bochum, Germany*
C.J. Umrigar - *Cornell University, USA*
A. Vittadini - *CNR, Padova, Italy*
W. Yang - *Duke University, USA*
J.L. Whitten - *NCSU, USA*

4.2 TMR Workshop

TMR-Network on 'Interface Magnetism'

Workshop on 'GMR'

in Dresden

September 12th - 14th, 1997

Purpose: Presentation and discussion of results and concepts to elucidate the microscopic origin of GMR and related phenomena

Arrival: Friday, September 12th, 1997

Departure: Sunday, September 14th, 1997 after lunch

We plan to have longer contributions (40 minutes) and short contributions (20 minutes) + discussion starting Friday late afternoon, Saturday and Sunday morning.

Requirements:

Please confirm your participation by sending me an e-mail and indicate the accompanying guests and any request concerning the accomodation until

August 24th, 1997.

Please fill in the following table and e-mail back to:

mertig@theory.phy.tu-dresden.de

Name:
Postal Adress:
telefon/fax:
e-mail:
share room with:
title of your contribution, if any:

Please send me a short abstract in latex form for each contribution, suitable to be presented in the Ψ_k – *Newsletter* until

August 31st, 1997.

Tentative list of participants:

	group	**name**
1	Eindhoven,Delft	G. Bauer
2		A. Bratas
3		P. Kelly
4		K. Scheep
5	Nagoya	J. Inoue
6	Vienna	C. Blaas
7		J. Kudrnovsky
8		L. Szunyogh
9		P. Weinberger
10		
11	Jülich	P.H. Dederichs
12		
13	Munich	H. Ebert
14		
15	Bremen	J. Banhart
16	Stockholm	D. Oberschmidt
17	Dresden	J. Binder
18		I. Mertig
19		P. Zahn

4.3 VI Italian-Swiss Workshop on COMPUTATIONAL MATERIALS SCIENCE

Dipartimento di Scienze Fisiche, Universitá di Cagliari Istituto Nazionale di Fisica della Materia, Cagliari Research Unit

19 - 23 September 1997

Hotel Costa dei Fiori, S. Margherita di Pula, Sardinia, Italy

An International Workshop on Computational Techniques and Applications to Materials Science

FORMAT: about 20 invited lectures, oral sessions for CONTRIBUTED papers (POSTER session possible depending on number of participants)

PROCEEDINGS: All contributions will be published in a special volume of the Conference Proceedings Series of the Italian Physical Society. Deadline for submitting contributions is August 15, 1997: contact V. Fiorentini at fiore@ciop.unica.it for info. Manuscripts will be due at the Workshop.

VENUE: Hotel Costa dei Fiori in S. Margherita di Pula (CA): an attractive sea resort on the south-western coast of Sardinia, providing comforts and an informal atmosphere.

GENERAL INFO: see below. For more details on registration contact the organizing secretariat at corsieco@mbox.vol.it For scientific queries contact fiore@ciop.unica.it. Also: check out the forthcoming on-line info at http://sparc10.unica.it

INVITED SPEAKERS (so far) AND TENTATIVE TITLES: (∗ to be confirmed)

F. ANCILLOTTO (Universitá di Padova)
High pressure phases of methane

G. BACHELET (Universitá di Roma-I)
Curvilinear coordinates for full-core atoms

F. BERNARDINI (Universitá di Cagliari)
Polarization and piezoelettricity effects at nitride interfaces

N. BINGGELI (EPF Lausanne)
GaAs/Al Schottky barriers

A. DAL CORSO (IRRMA Lausanne)
CO vibrations on Cu surfaces

∗ A. GARCIA (Universidad del Pais Vasco, Bilbao)
Dislocations in ferroelectric $BaTiO_3$

P. GHOSEZ (Universite de Louvain)
Dynamical charges and stability in ferroelectrics

H. KRAKAUER (College of William and Mary, Williamsburg)
title to be announced (topic: ferroelectrics)

J. L. MARTINS (INESC Lisboa)
A new variable-cell-shape molecular dynamics

M. METHFESSEL (IHP Frankfurt/Oder)
Forces in the FP-LMTO method: formalism and applications

A. PASQUARELLO (IRRMA Lausanne)
Ab initio study of quartz amorphization

P. PAVONE (Universitaet Regensburg)
Ab initio surface phonons in semiconductors and semimetals

R. RESTA (Universitá di Trieste)
Topics in polarization theory

P. VOGL (Schottky Institute, Munich)
High field transport in nitride-based devices Exact exchange formalism for LDA calculations

∗ W. WEYRICH (Universitaet Konstanz)
title to be announced (topic: measurement of density matrices)

REGISTRATION

Please send registration form (accompanied by payment receipt) by fax preferrably before July 31 1997 to

Corsi & Congressi,
via Galassi 2, I-09131 Cagliari
tel/fax: +39 70 522777

CONFERENCE FEE including lodging full-board at Hotel Costa dei Fiori from dinner on 18/9 to breakfast on 24/2, coffee breaks, evening refreshments, etc., is:

double room lodging ⇒ Italian Lire 860000 (∼500 US $)
single room supplement ⇒ Italian Lire 250000 (∼160 US $)

PAYMENT should be effected by bank money transfer on the bank account No. 11080620154 of Corsi& Congressi, at Banca Commerciale Italiana, Sede di Cagliari, Codice ABI 2002 - CAB 43950.

Registration form

Name .....
Institution .....
e-mail address .....
Arrival date:.../.../97 - Departure date:.../.../97
Accomodation: Single room [...] Double room [...]
Would share double room with .....
Plan to present contributed talk/poster: [...]

Series Chairman : prof. A. Baldereschi - EPFL Lausanne
Workshop Chairman : prof. F. Meloni - INFM and Universita' di Cagliari
Scientific Secretary: dr. V. Fiorentini - INFM and Universita' di Cagliari

Ph.D. Position in Photonic Band Structures

Max-Planck-Insititute of Microstructure Physics and Martin-Luther-University Halle-Wittenberg, Germany

A position in the field of photonic crystals in the department of Professor U. Goesele (MPI), is currently available for a Ph.D student (A 13/2), starting on October 1 (or later this year) at the above mentioned Institutes. The position is expected to last two years; but may be extended to three. In addition to our experimental work done with photonic crystals, theoretical calculations and interpretations will be made on the pho- tonic band structures of these materials. The subject of the thesis will involve the methodical and theoretical study of band structure calculations of defect structures in photonic crystals, together advised by Prof. W. Hergert (Univ. Halle) and Dr. R. Hillebrand (MPI Halle).

Applicants should have successfully passed the diploma exams in Physics and have reasonable working experience with computers and programming. A good academic background in solid state physics and experience with band structure calculations is desired. Women are encouraged to apply for the job. Disabled individuals will be preferred if comparably suited for the position.

Please, contact for application:

Prof. W. Hergert, Martin-Luther-Universitaet Halle-Wittenberg, Fachbereich Physik, Fachgruppe Theoretische Physik, D-06099 Halle
email : hergert@physik.uni-halle.de

or

Dr. R. Hillebrand, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle.

Post-doctoral position at the University of Missouri in Electronic Structure Theory

Applications are invited for a post-doctoral position in the area of Electronic Structure of Magnetic Materials. Experience in the area of magnetism theory and in density-functional methods, such as full-potential and ASA LMTO methods, is desirable. The position is available beginning September 1, 1997 for one year and may be extended subject to availability of funds. The University of Missouri has a vibrant research program in Condensed Matter Theory and Experiment. Interested candidates should send a resume and arrange to have three letters of recommendation sent to: **Prof. S. Satpathy, Department of Physics, University of Missouri, Columbia, MO 65211, USA**. The University of Missouri is an equal opportunity/affirmative action employer. Minorities and women are especially urged to apply.

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

6 New TMR Network

The TMR network proposal: 'Electronic Structure calculations of materials properties and processes for industry and basic science' has been favourably evaluated by the EU Commission, and it is close to certain that the final contract negotiations will be finished this autumn.

This means that the network will be launched early spring 1998, with a duration of 3 or 4 years. Associated with the network are **8 post-doc positions** each of a duration of 2 1/2 - 3 years. The rules are that a post-doc position in a given EU country cannot be filled by a person from that same country. It must be filled by a person from another EU country or from one of the countries associated with the TMR program (Iceland, Norway, Israel and Liechtenstein). The 8 post-doc positions likely to be negotiated through the EU Commission are dedicated to the following tasks (researcher in charge is also quoted with email address):

1. Molecular processes on oxide surfaces.
   Paris, France. Dr. E. Wimmer; ewimmer@msi.fr

2. Self-Interaction Correction calculations on f-electron systems.
   Aarhus, Denmark. Dr. A. Svane; svane@dfi.aau.dk

3. Oxide interfaces and surfaces.
   Belfast, UK. Prof. M. Finnis; m.finnis@qub.ac.uk

4. Oxide interfaces and surfaces.
   Keele, UK. Prof. M. Gillan; pha71@cc.keele.ac.uk

5. Non-collinear magnetism.
   Vienna, Austria. Prof. J. Hafner; jhafner@tph.tuwien.ac.at

6. Molecular dynamics with LAPW.
   Jülich, Germany. Dr. S. Blügel; s-bluegel@kfa-juelich.de

7. Electron excitations and optical properties.
   Helsinki, Finland. Prof. R. Nieminen; rniemine@csc.fi

8. Superconductivity.
   Würzburg, Germany. Prof. E. K. U. Gross; gross@physik.uni-wuerzburg.de

If you are interested in more details, please contact the rsearcher listed (or myself!) for further information.

Network Coordinator
Axel Svane
svane@dfi.aau.dk

7 Abstracts

Interlayer exchange coupling: effect of the cap

J. Kudrnovský and V. Drchal
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and
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P. Bruno
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P. Weinberger
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Getreidemarkt 9, A-1060 Vienna, Austria

Abstract

The effect of non-magnetic cap-layers on the periods, the amplitudes, and the phases of the oscillations of interlayer exchange coupling (IEC) is studied theoretically using *ab initio* methods. We employ the spin-polarized surface Green function technique within a tight-binding linear muffin-tin orbital method and the Lloyd formulation of the IEC. Application is made to Co/Cu/Co(001) trilayers with a Cu-cap interfacing vacuum through the dipole barrier. We investigate in detail both an asymmetric case with one semiinfinite Co-slab and the other Co-slab being five monolayers thick and a symmetric case with Co-slabs of monolayer thickness. In all cases we have found a pronounced oscillatory behavior of the amplitudes and the phases of the IEC oscillations as a function of the thickness of the cap. The case of different spacer- and cap-materials is also studied. The results for different spacer and different cap thicknesses are analyzed in terms of a discrete Fourier transformation as well as in real space, and found to confirm predictions by the electron confinement model on an *ab initio* level.

(Submitted to Phys. Rev. B)
Manuscripts available from: pw@ws1.cms.tuwien.ac.at

This paper acknowledges the TMR-Network on 'Interface Magnetism'.

Oscillatory behavior of the magnetic anisotropy energy in Cu(100)/Co_n multilayer systems

L. Szunyogh[a,b], B. Újfalussy[a], C. Blaas[c],
U. Pustogowa[a], C. Sommers[d] and P. Weinberger[a,c]

[a] *Center for Computational Materials Science, Vienna, Austria*

[b] *Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary*

[c] *Institut für Technische Elektrochemie, Technische Universität Wien, Vienna, Austria*

[d] *Laboratoire de Physique des Solides, Campus d'Orsay, Orsay, France*

Abstract

The oscillatory behavior of the magnetic anisotropy energy in different types of Co_n multilayers on a Cu(100) substrate, including free surfaces, capped surfaces and Co/Cu spacer systems, is shown in terms of ab-initio like calculations using the selfconsistent fully relativistic spin-polarized Screened Korringa-Kohn-Rostoker method. Deduced from direct representations and discrete (linear) Fourier transformations with respect to the number of Co layers, a period of two monolayers seems to be characteristic for these oscillations, whereas for a given number of Co layers and viewed with respect to the number of Cu spacer layers they rapidly approach the value of the magnetic anisotropy energy for the corresponding Co_n multilayer on Cu(100) with a semi-infinite Cu cap, the so-called biased value. By excluding the so-called preasymptotic regime a short and a long period of 2.5 and 5.5 monolayers, respectively, can be traced for the oscillations with respect to the number of Cu spacer layers.

All types of oscillations, namely either with respect to the number of Co layers or with respect to the number of Cu spacer layers, are analyzed in terms of layer-resolved band energy contributions to the magnetic anisotropy energy. Such a layer-wise distribution of the magnetic anisotropy energy not only allows one to characterize different regimes of thicknesses, but also to discuss the effect of the actual interface on the absolute values of the magnetic anisotropy energy, shown in particular by considering a system with Co/Au interfaces.

(Submitted to Phys. Rev. B)

Manuscripts available from: pw@ws1.cms.tuwien.ac.at

This paper acknowledges the TMR-Network on 'Interface Magnetism'.

Effect of cap-layers on interlayer exchange coupling

J. Kudrnovský[a,b], V. Drchal[a,b], P. Bruno[c], R. Coehoorn[d],
J.J. de Vries[d,f], K. Wildberger[e], P.H. Dederichs[e], and P. Weinberger[b]

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and

[b] *Center for Materials Science, Technical University, A-1060 Vienna, Austria*

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[e] *Forschungszentrum Jülich, IFF, D-52425 Jülich, Germany*

[f] *Eindhoven University of Technology, NL-5600 MB Eindhoven, The Netherlands*

Abstract

The effect of non-magnetic cap-layers on the amplitudes and the phases of the oscillations of interlayer exchange coupling (IEC) is studied theoretically on *ab initio* level. We employ a spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method and the Lloyd formulation of the IEC. Application is made to Co/Cu/Co(001) trilayers with Cu-cap layers interfacing vacuum through the dipole barrier.

(Proceedings of the MRS Spring Meeting '97, San Francisco)
Manuscripts available from: pw@ws1.cms.tuwien.ac.at

This paper acknowledges the TMR-Network on 'Interface Magnetism'.

Oscillatory behavior of interface exchange coupling caused by finite caps of variable thickness

J. Kudrnovský[a,b], V. Drchal[a,b], P. Bruno[c], I. Turek[d],
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[d] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic*

Abstract

The effect of non-magnetic cap-layers on the periods and the amplitudes of the oscillations of interlayer exchange coupling (IEC) is studied theoretically using an *ab initio* spin-polarized surface Green function technique within a tight-binding linear muffin-tin orbital method and the Lloyd formulation of the IEC. Applications are made to the free-electron like model as well as to Co/Cu/Co(001) trilayers with a cap interfacing vacuum through the dipole barrier. The results are analyzed in terms of a discrete two-dimensional Fourier transformation which confirms a pronounced oscillatory behavior of the IEC with respect to the thickness of the cap and the spacer layers. The results are in agreement with available experimental data as well as with predictions of the electron confinement model of the IEC.

(Proceedings of the ICAM '97/E-MRS Spring Meeting, Strasbourg 1997)
Manuscripts available from: pw@ws1.cms.tuwien.ac.at

This paper acknowledges the TMR-Network on 'Interface Magnetism'.

What is "non-collinear magnetism"?

P. Weinberger
Institut für Technische Elektrochemie
and
Center for Computational Materials Science
Technical University of Vienna
Getreidemarkt 9/158, A-1060 Vienna, Austria

Abstract

The terms "collinear" and "non-collinear" refer originally to a geometrical concept. Nowadays they are frequently used to classify magnetism in a rather vague sense. In the present paper an attempt is made to classify "collinear" and "non-collinear" by means of transformation properties of "classical vectors" (Heisenberg-like models of magnetism), and "spinors" and "bispinors" as used within a non-relativistic and a relativistic description of magnetism based on the (local) density functional approach.

- In: *"Current Problems in Condensed Matter: Theory and Experiments"*, Ed.: J. L. Moran-Lopez, Plenum Press.
- This paper is dedicated to Prof. Karl-Heinz Bennemann on occasion of his 65th birthday.

Manuscripts available from: pw@ws1.cms.tuwien.ac.at

Band picture of the spin-Peierls cuprate $CuGeO_3$

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Laboratory for Theoretical Physics and Physics of Condensed Matter (020),
Institute of Nuclear Sciences – "Vinča",
P.O. Box 522, 11001 Belgrade, Yugoslavia

Abstract

The electronic structure for the cuprate $CuGeO_3$ has been studied by the generalization of the local-density-approximation method for the systems with strong Coulomb correlations. The stable insulating antiferromagnetic solution with energy gap of ~ 3.02 eV and magnetic moment of 0.89 μ_B is obtained for the first time. According to our results the strong copper on-site Coulomb interaction of U=9.66 eV is the most important quantity for the gap openning in this first inorganic spin-Peierls compound discovered recently.

(Submitted to Phys. Rev. B.)
Manuscripts available from: zeljkos@rt270.vin.bg.ac.yu

Coulomb correlated band structure of one dimensional $SrCuO_2$

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Laboratory for Theoretical Physics and Physics of Condensed Matter (020),
Institute of Nuclear Sciences – "Vinča",
P.O. Box 522, 11001 Belgrade, Yugoslavia

Abstract

The spin-restricted, spin-polarized, and LDA+U fully self-consistent linear muffin-tin orbital band structure for "one-lag ladder" compound $SrCuO_2$ has been studied. The extremely small band gap solution with negligible magnetic moment on Cu sites is obtained in the framework of LSDA method. On the other hand, the LDA+U method have produced the insulating antiferromagnetic solution with energy gap of 1.63 eV and magnetic moment of $0.89\mu_B$. The standard LDA and LSDA $SrCuO_2$ bands around the Fermi level are so similar to the recently discovered spin-Peierls inorganic compound $CuGeO_3$ that one could perhaps expect the appearance of the same type of phase transition in orthorhombic strontium copper oxide $SrCuO_2$.

(Submitted to Phys. Rev. B (Rapid Communications))
Manuscripts available from: zeljkos@rt270.vin.bg.ac.yu

First principles investigations of a "quasi-1-dimensional" charge transfer molecular crystal: TTF-2,5Cl_2BQ

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Abstract

We performed first-principles calculations using the projector augmented wave method in order to get a clear description at a microscopic level of the electronic distribution far from the transition for TTF-2,5Cl_2BQ. Our calculations predict for the first time a low-symmetry structure (ground state) of this compound. We relate them to a simple tight-binding scheme which allows us to discuss the pertinence of the 1-dimensional models used to study the phase transitions in this class of materials.

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Theoretical approaches of magnetism of transition metal thin films and nanostructures on semi-infinite substrate

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Abstract

Tremendous progress has been made in the field of magnetic materials and technology over the past few years. Superior properties and novel scientific questions arise from our ability to either synthetize artificial structures or tailor microstructures at the appropriate length scale. The study of low-dimensional magnetism of thin films, surfaces and interfaces has revealed new and sometimes unexpected properties. In this review we focus on the determination of the local magnetic moments distribution at the surface of transition metals, for very thin transition metal films and nanostructures on noble and transition metal substrates at T=OK.

Two different approaches are commonly used. Ab-initio and semi-empirical tight binding calculations appear to be complementary to determine the electronic structure. The first provides very precise results for periodically ordered systems, whereas the second is able to study complex systems with a large number of inequivalent sites. We discuss these approaches and point out recent development which combines the versatility of the ab-initio method with the rapidity of the tight-binding calculation. Special attention is devoted to the magnetic frustration which occurs when both ferromagnetic and antiferromagnetic couplings are present. The Fe/Cr interface which has been, since ten years, one of the most studied system is a good exemple.

Recent experimental and theoretical efforts have addressed the question of a possible onset of ferro-or antiferromagnetism in nanostructures, free-standing clusters, thin-film structures of metals that are non-magnetic in the bulk form. V, Pd, Rh and Ru have been singled out as potential candidates. Thus particular attention will be devoted for V free-standing films, as well as V monolayer on Ag and Fe. Rh and Ru have been found magnetic experimentally in the form of cluster (Rh) and for Ru monolayer on graphite. However Rh monolayer on Ag is found experimentally non-magnetic whereas calculations show that magnetism is killed when surface alloy is considered. Pd is another important element to consider because, being non-magnetic in the atomic form as well as in bulk form it present high susceptibility. Therefore it can become magnetic if its lattice parameter is slightly increased. It is believed to be magnetic in the case of a bilayer on Ag(001). Induced polarization is obtained when Pd is in contact with a magnetic metal.

Because of its exotic structural and magnetic properties, Mn is an interesting candidate for thin-film growth as it is expected to accept different local configurations. Experimentally, one may attempt to stabilize normally high-temperature phases of Mn by epitaxial growth on a suitable substrate. We will show that Mn takes on the c(2x2) magnetic configuration for the Mn monolayer on Fe(001) and Co(001).

Calculations show that Ir and Pt, in the monolayer range, are magnetic when grown on Ag. However, no experiment has displayed any kind of magnetism yet and more realistic

calculation has shown that spin-orbit effect kills the magnetic moment. Therefore only V, Cr, Mn, Co and Ni for 3d, and Ru, Rh and Pd for 4d will be considered in this review.

(Surface Science Reports, in press)
Manuscripts available from: hugues@lugh.u-strasbg.fr

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Complex magnetic behavior at the surface of B2 ordered FeCr alloy

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Abstract

Bouzar et al have recently investigated the surface of B2 FeCr alloy. In all cases of crystal growth <001>, <110> and <111> they found the local polarisation at the surface to be antiferromagnetically coupled with the subsurface layer in contrast to parallel coupling between Fe and Cr in bulk FeCr. In order to assert these results, we have investigated the local polarization of Fe at the (001) surface of this alloy with a Tight-Binding Linear Muffin Tin Orbitals model. Using general gradient approximation with Langreth-Mehl-Hu functional for $p(1 \times 1)$ and $c(2 \times 2)$ configurations we found the local polarisation at the Fe surface layer to be antiferromagnetically coupled with the subsurface Cr layer and high magnetic moments compared to the bulk values.

(Computational Materials Science, in print)
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Metalicity, susceptibility and superconductivity in A_3C_{60} (A= K, Rb)

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Abstract

We study the condition for a Mott-Hubbard metal-insulator transition. We find that the orbital degeneracy N shifts the critical value of the Coulomb interaction where the transition takes place by a factor of the order of $\sqrt{N}$. This explains why A_3C_{60} (A= K, Rb) are metals. We furthermore calculate the Pauli susceptibility χ. From the calculated many-body enhancement and experimental values of χ, we deduce the density of states. Finally, we discuss the strength of the electron-phonon interaction and the superconductivity.

(Proceedings of the 191st Electrochemical Society Meeting, Montreal, 1997;
J. Electrochem. Soc.)
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Discrete Hubbard-Stratonovich transformations for systems with orbital degeneracy

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Abstract

A discrete Hubbard-Stratonovich transformation is presented for systems with an orbital degeneracy N and a Hubbard Coulomb interaction without multiplet effects. An exact transformation is obtained by introducing an external field which takes $N+1$ values. Alternative approximate transformations are presented, where the field takes fewer values, for instance two values corresponding to an Ising spin.

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Superconductivity in doped C_{60} compounds

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Abstract

It is discussed why A_3C_{60} (A =K, Rb) are metals and not Mott-Hubbard insulators, in spite of the strong Coulomb repulsion U. It is shown that the orbital degeneracy N of the t_{1u} band increases the critical value of U for a Mott-Hubbard transition by about a factor of $\sqrt{N}$. Theoretical and experimental estimates of the electron-phonon coupling λ are discussed. In particular, it is shown how photoemission for free C_{60}^- molecules can be used to estimate λ. Finally we discuss the Coulomb pseudopotential μ^*, describing the effects of the Coulomb repulsion. In particular the retardation effects are considered. It is argued that μ^* is relatively large, but that the results are still consistent with the electron-phonon interaction driving the superconductivity.

(Proceedings of "Pair Correlation in Many-Fermion Systems", Erice, 1997)
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Relativistic and non-relativistic electron transport in disordered alloys: I. Theory

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Abstract

The electrical conductivity of disordered alloys is calculated using the Korringa-Kohn-Rostoker–coherent potential approximation (KKR–CPA) alloy theory in conjunction with the local density approximation to density functional theory and the Kubo-Greenwood equation. Relativistic and non-relativistic expressions for the conductivity are derived. A technique for the evaluation of the Kubo-Greenwood equation for arbitrary crystal symmetry using group theoretical methods is described. Explicit expressions for scattering and current operators at complex energies below the real axis which occur in the evaluation of the Kubo-Greenwood equation are given.

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Relativistic and non-relativistic electron transport in disordered alloys. II. Application to palladium alloyed with copper, silver, and gold

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Abstract

The residual electrical dc resistivity of the transition metal alloy systems Cu–Pd, Ag–Pd, and Au–Pd was calculated by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR–CPA) for the solution of the electronic structure problem and the one-electron Kubo–Greenwood formula for the conductivity calculations. All systems were treated on a non-relativistic and a scalar relativistic level in order to be able to assess the importance of some of the relativistic effects. For one alloy also a fully relativistic calculation was performed thus allowing to give an estimate for the spin-orbit induced contributions neglected in the scalar relativistic approach. The calculated concentration dependent resistivities were compared to corresponding experimental values. The electrical resistivity (or conductivity) is decomposed into angular momentum and k-resolved quantities. This allows for a discussion of the origin of electronic conduction in the alloys considered. Energy-dependent conductivities with and without vertex corrections permit a discussion of the importance of vertex corrections. The results for the Kubo-Greenwood equation without vertex corrections are compared to results obtained using the semiclassical Boltzmann equation in the relaxation time approximation.

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Optical properties of monoclinic SnI_2 from relativistic first principles theory

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Abstract

Within the local density approximation, using the relativistic full potential linear muffin-tin orbital method (FPLMTO), the electronic structure is calculated for the anisotropic, layered material SnI_2. The direct interband transitions are calculated using the full electric-dipole matrix elements between the Kohn-Sham eigenvalues in the ground state of the system. The inclusion of spin-orbit coupling was found to change the optical properties of this material considerably. Polarized absorption and reflectionspectra are calculated and compared with recent experimental results. The experimentally suggested cationic excitation for the lowest energy transition is confirmed. From the site and angular momentum decomposed electronic structure studies and the detailed analysis of the optical spectra it is found that the lowest energy transition is taking place between Sn5s (atom type 2a) $\rightarrow$ Sn5p (atom type 4i) states. The ground state calculation was repeated using the tight-binding LMTO-ASA method, and the resulting bandstructure agrees very well with the one calculated with the full-potential method. In contrast to recent experimental expectation, our calculations show an indirect bandgap, which is in agreement with earlier semiempirical tight-binding calculations as well as with absorption and reflection spectra.

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Interfacial alloying and interfacial coupling in Cr/Fe(001)

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Abstract

The magnetic order of Cr layers on Fe(001) is studied taking into account interfacial alloying and possible interdiffusion. The interfacial alloy is modelled by either a one-monolayer or a two-monolayer ordered compound whose concentration is varied. The spin-polarized electronic structure is determined self-consistently by solving a *d*-band tight-binding hamiltonian. We determine the concentration for which the phase of the layer-by-layer antiferromagnetic structure of Cr changes in the Cr film on Fe(001). We find that in the case of two interfacial mixed layers, a π phase shift occurs at a Cr concentration between 33% and 50% when 3 monolayers (ML) of Cr are deposited. This π phase shift changes to a concentration between 11% and 25% for a more important coverage of Cr (namely 11 ML). When only one mixed layer is considered, the phase of the antiferromagnetic stacking of Cr changes at a concentration between 25% and 33% for 3 ML of Cr and between 33% and 50% for 11 ML of Cr. A simulation of the variation of the magnetization during Cr growth shows that the more Cr and Fe are interdiffused at the interface, the more important is the decrease of the magnetization. We compare our results to the many experimental data available.

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Inverse versus Normal NiAs Structures as High Pressure Phases of FeO and MnO

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Abstract

Intensive high-pressure experiments on the transition-metal monoxides have revealed that FeO and MnO undergo pressure-induced phase transition. The high-pressure phase of FeO was identified as the NiAs (B8) type, while that of MnO is yet unclear. The present theoretical study predicts that the high-pressure phase of MnO is a metallic normal B8 structure (nB8), while that of FeO should take the inverse B8 structure (iB8). The novel feature of the unique high-pressure phase of stoichiometric FeO is that the system should be a band insulator in the ordered antiferromagnetic (AF) state and that the existence of a band gap leads to special stability of the phase. The observed metallicity of the high-pressure and high-temperature phase of FeO may be caused by the loss of AF order and also by the itinerant carriers created by non-stoichiometry. Analysis of x-ray diffraction experiments provides a further support to the present theoretical prediction for both FeO and MnO. Strong stability of the high-pressure phase of FeO will imply possible important roles in Earth's core.

(Submitted to Nature)

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Magnetism of epitaxial Ru and Rh monolayers on graphite

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Abstract

Recently, Pfandzelter et al. reported the first observation of monolayer ferromagnetism of a $4d$ metal, namely in a Ru monolayer grown on graphite. Using the tight-binding linear-muffin-tin-orbital method we have calculated the electronic and magnetic structure of epitaxial Ru and Rh monolayers on graphite with the experimentally determined atomic density. Monolayers of the other $4d$ elements were found to be non-magnetic already in the free–standing limit. The magnetic structure of the Ru and Rh monolayers is studied as a function of metal–graphite interlayer distance h. They become magnetic at $h = 4.5$ a.u. (Ru) and $h = 4.8$ a.u. (Rh) in a first order transition. In the assumed $p(2\times 2)$ super–structure, the moments on the "hollow" site atoms are up to four times bigger than those on the "on-top" site atoms. For $h > 5.4$ a.u. (Ru) and $h > 5.1$ a.u. (Rh) the site dependence vanishes and the moments of the free monolayers are approximately reached (1.9 $\mu_{\rm B}$ and 1.2 $\mu_{\rm B}$, respectively).

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Dipole waves in semiconductors: the dielectric function and plasma oscillations of silicon

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Abstract

The relationship between bond polarisability, local fields and the dielectric function of bulk silicon is investigated using the discrete dipole model. In this model a valence electron pair (a bond) is treated as a point-like polarisable unit which responds to the local field at the bond by creating a dipole moment there. We assume an unretarded form for bond-bond interactions (local fields) and find the normal modes of an infinite lattice of bonds with the diamond structure. We call these normal modes dipole waves and express the dielectric function for bulk silicon in terms of them. Dipole waves corresponding to optical transitions and bulk plasma oscillations are identified and it is shown that the experimental peak positions and intensities in both the dielectric function and dielectric loss function of silicon are reproduced by this model. The form of bond-bond interaction chosen is the electrostatic interaction between point-like dipoles but this approximation breaks down at short range. Bond-bond interactions at short range and bond polarisabilities are therefore calculated from ab initio cluster calculations. The static dielectric function is obtained as a function of bond polarisability using point dipolar fields and local fields corrected at short range for the finite size of a bond. Comparison is made with the Clausius-Mossotti relationship between dielectric function and polarisability.

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Reflectivity and reflectance anisotropy of Si(100): a polarisable bond model

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Abstract

The reflectivity and reflectance anisotropy (RA) of the unreconstructed Si(100) surface are calculated using a model in which the semiconductor is a slab of polarisable bonds interacting by induced dipolar fields. Parameters for the calculations are obtained from ab initio calculations. The dielectric response of the slab is analysed in terms of dipole-moment normal modes which are called dipole waves. At the gamma-bar point of the surface Brillouin zone, dipole waves are polarised either parallel or perpendicular to the surface. We find that the normal incidence reflectivity of the dipole lattice reproduces the magnitude of the experimental reflectivity of silicon in the energy range 1-6 eV but lacks spectral features. Local fields near the surface of the slab differ from local fields in the bulk, and consequently the surface of the slab responds to optical radiation at a slightly higher frequency than the bulk, and the slab has a maximum RA of the order of 0.7and the experimental RA spectra of the Si(100)-(2x1) and Si(100)-(2x1)-As surfaces.

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Local stability of higher-energy phases in metallic materials and its relation to the structure of extended defects

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Abstract

Relative structural stability of elemental cubic transition metals and some transition metal aluminides with respect to tetragonal and trigonal deformation is investigated. Total energy calculations show that all higher-energy cubic structures studied are locally unstable with respect to at least one of those deformation modes. In intermetallics, there may or may not be symmetry-dictated energy extrema corresponding to cubic lattices depending on the atomic ordering. However, other energy extrema along the deformation paths besides those required by symmetry occur. Configurations corresponding to energy minima on the transformation paths may represent metastable structures that can play an important role in interfaces and other extended defects.

(Comput. Mat. Sci. **8** (1997), 100-106)
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Atomic configuration and electronic structure of extended defects from the point of view of positron annihilation: A grain boundary example

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Abstract

A quantum-mechanical approach for determining the electronic structure and atomic configuration of extended defects in metals is described and importance of theoretical methods for interpretation of positron annihilation spectroscopy data is stressed. The electronic structure in defect region is calculated employing the self-consistent Green's function approach based on the tight-binding linear muffin-tin orbital (TB-LMTO) method within the atomic-sphere approximation (ASA). For atomic relaxation, we use (i) Finnis-Sinclair type many-body central force potentials and (ii) a recently developed quantum-mechanical method in which the angular dependence of interatomic forces is properly accounted for. In the latter case, the Hamiltonian is constructed within the TB-LMTO-ASA approach as well. As an example, atomic configuration of the $\Sigma = 5(210)/[001]$ tilt grain boundary in tungsten is determined and local densities of states at atoms in defect region are discussed.

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Preferential positron annihilation in Fe-Al system

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Abstract

The effect of preferential positron annihilation in binary Fe-Al system is studied by means of the LMTO electron and positron structure method. The study covers the whole concentration range from Fe to Al. The supercell approach is utilized to model the structure of alloys. We conclude that positron preferential occupation of Fe sites is negligible for small Al concentrations and increases with Al content. The effect of positron preferential annihilation at Fe sites is also negligible, if there is any. The non-linear dependence of positron annihilation rate on Al concentration can be almost fully explained as a volume effect.

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Detection of Ti-rich precipitates in iron by means of positron annihilation spectroscopy

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Abstract

A possibility of detection of various Ti-rich precipitates in iron (steels) using positron annihilation spectroscopy is analyzed. First, we investigate precipitates with sulphur (Ti_9S_9, $Ti_4C_2S_2$), which have not been studied yet. Then, the comparison with already examined TiC and TiN systems is performed. We use the ab initio LMTO method and calculate positron affinities of all studied perfect systems. We also employ an improved supercell technique and atomic superposition method and determine positron lifetimes for systems with vacancies. It turns out that even undefected Ti_9S_9 and $Ti_4C_2S_2$ precipitates can bind a positron and, therefore, may be detected in positron annihilation experiments in contrast to TiC and TiN precipitates which can trap positrons only if they contain vacancies.

(Nukleonika **42** (1997), 143-152)
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Magnetically Stabilized Surface Alloys

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Abstract

We investigate the interrelation of magnetism and stability of ultrathin magnetic films and come to the conclusion that under certain circumstances there should exist magnetically stabilized two-dimensional surface alloys. We present *ab initio* results for the formation energy and the interdiffusion energy of Cu(001)c(2×2) 3*d* surface alloy films. Results based on the density functional theory in the local spin density approximation (LSDA) indicate the existence of a thermodynamically stable surface alloy: Cu(001)c(2×2) Mn. Although in detail, the results depend on the Cu substrate, the trends presented below have an universal character. Therefore, Cu(100)c(2×2)Mn is only an example of a much wider class of magnetic surface alloys. Recently, several of these surface alloys have been found experimentally, showing an unexpectingly large structural corrugation of the surface alloy atoms. This will be discussed as an results of a large magneto-volume effect. We found in addition a nonmagnetic surface alloy Ti/Cu(001), which is not yet confirmed experimentally. Total energy calculations are carried out using the full–potential linearized augmented planewave (FLAPW) method in film geometry.

(Appl. Phys. A **63**, 595 (1996).)
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Effect of lattice distortions on the competition between the double and superexchange mechanisms in $LaMnO_3$

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Abstract

Double exchange (DE), superexchange (SE) and higher ordercontributions to the exchange interaction energy between Mn layers in $LaMnO_3$ are studied using the linear-muffin-tin-orbitals method as generalized to treat non-collinear magnetic configurations.The degree of the internal lattice distortion (f) and the angle (θ) between ferromagnetically ordered Mn layers are considered as simulation parameters . We find that both global and internal lattice distortions dramatically influence the character of the exchange interactions: globaldistortions associated with variations of the apical Mn-O bond length promotes the DE contribution; the bending of the Mn-O bonds in the (a-b) plane suppresses the DE and promotes the antiferromagnetic SE contribution to the interlayer exchange energy. Overall, the character of exchange interactions is determined by SE contributions: in hypothetical FM phases DE interactions mediated by itinerant electrons is present but still rather small compared with SE; in AFM phases this DE is negligible and non-Heisenberg terms are small compared with SE.

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Manuscript available from: onm@saturn.phys.nwu.edu

Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange-correlation

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Abstract

In *ab initio* pseudopotential calculations within density-functional theory the nonlinear exchange-correlation interaction between valence and core electrons is often treated linearly through the pseudopotential. We discuss the accuracy and limitations of this approximation regarding a comparison of the local density approximation (LDA) and generalized gradient approximations (GGA), which we find to describe core-valence exchange-correlation markedly different. (1) Evaluating the binding properties of a number of typical solids we demonstrate that the pseudopotential approach and namely the linearization of core-valence exchange-correlation are both accurate and limited in the same way in GGA as in LDA. (2) Examining the practice to carry out GGA calculations using pseudopotentials derived within LDA we show that the ensuing results differ significantly from those obtained using pseudopotentials derived within GGA. As principal source of these differences we identify the distinct behavior of core-valence exchange-correlation in LDA and GGA which, accordingly, contributes substantially to the GGA induced changes of calculated binding properties.

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Island morphology and adatom self-diffusion on Pt(111)

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Abstract

The results of a density-functional-theory study of the formation energies of (100)- and (111)-faceted steps on the Pt(111) surface, as well as of the barrier for diffusion of an adatom on the flat surface, are presented. The step formation energies are found to be in a ratio of 0.88 in favour of the (111)-faceted step, in excellent agreement with experiment; the equilibrium shape of islands should therefore clearly be non-hexagonal. The origin of the difference between the two steps is discussed in terms of the release of stress at the surface through relaxation. For the diffusion barrier, we also find relaxation to be important, leading to a 20% decrease of its energy. The value we obtain, 0.33 eV, however remains higher than available experimental data; possible reasons for this discrepancy are discussed. We find the ratio of step formation energies and the diffusion barrier to be the same whether using the local-density approximation or the generalized-gradient approximation for the exchange-and-correlation energy.

(submitted to Phys. Rev. B)
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Shape and stability of quatum dots

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Abstract

The formation of dislocation-free three-dimensional islands by heteroepitaxial growth of lattice mismatched materials is utilized to produce partially ordered arrays of quantum dots. The shape of these islands results from the competition between surface and elastic energies. We have studied the system InAs/GaAs (110) in detail. InAs surface energies have been computed *ab initio* for several orientations and the elastic energy of the islands has been calculated within a continuum theory. The resulting equilibrium islands are hills bounded by {110}, {111} and $\{\bar{1}\bar{1}\bar{1}\}$ facets and a (001) surface on top. We compare to experiment and discuss the influence of growth kinetics on the shape.

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Maximally-localized generalized Wannier functions for composite energy bands

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Abstract

We discuss a method for determining the optimally-localized set of generalized Wannier functions associated with a set of Bloch bands in a crystalline solid. By "generalized Wannier functions" we mean a set of localized orthonormal orbitals spanning the same space as the specified set of Bloch bands. Although we minimize a functional that represents the total spread $\sum_n \langle r^2 \rangle_n - \langle \mathbf{r} \rangle_n^2$ of the Wannier functions in real space, our method proceeds directly from the Bloch functions as represented on a mesh of k-points, and carries out the minimization in a space of unitary matrices $U_{mn}^{(\mathbf{k})}$ describing the rotation among the Bloch bands at each k-point. The method is thus suitable for use in connection with conventional electronic-structure codes. The procedure also returns the total electric polarization as well as the location of each Wannier center. Sample results for Si, GaAs, molecular C_2H_4 and LiCl will be presented.

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Influence of the alloy composition and local environment on the magneto-optical properties of Co_xPd_{1-x} alloys

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Abstract

Results of *ab-initio* calculations performed to investigate the dependence of magneto-optical properties of Co_xPd_{1-x} alloys on chemical ordering and alloy composition are presented. A new procedure of averaging the calculated spectra for compounds with respect to the orientation dependence of the gyration vector is proposed which makes it possible to account for the effects of random orientation of microcrystals in polycrystalline samples. Good agreement between theoretical and experimental spectra for varying alloy composition is found demonstrating the applicability of the theoretical approach.

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Influence of disorder on the magneto-optical properties of FePt

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Abstract

A scheme to deal with the magneto-optical properties of randomly disordered alloys is presented. This aim is achieved by calculating the optical conductivity tensor $\boldsymbol{\sigma}(\omega)$ for a number of ordered model compounds that differ in their atomic configuration within the unit cell but not in their composition. In a subsequent step the orientational and configurational average $\langle\boldsymbol{\sigma}(\omega)\rangle$ is taken. The magneto-optical properties are derived then from this in the conventional way. As it is demonstrated for FePt this approach accounts for the the influence of disorder on its magneto-optical in a very satisfying way.

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Applying Ab Initio Calculations in Mineralogy

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There are at least five university departments of Earth Sciences in Britain where some ab initio simulations are being carried out on minerals, and a few more university and other institutions in the rest of the world. The number of people involved in ab initio calculations of silicates and related phases becomes larger if one includes chemists making calculations on zeolite catalysts, a few zeolites being in fact minerals. There are also others, often physicists, who have done calculations on quartz and other simple silicates as test or demonstration calculations rather than being focused on solving specific mineralogical problems. One can therefore discern an embryonic community of ab initio computationalists beginning to make a contribution in mineralogy. Incidentally a mineral is any material occurring naturally in the earth. Minerals include many phases with very complex structure and crystal chemistry, particularly among the aluminosilicates, and including some of interest in materials science in connection with high performance ceramics.

How can ab initio calculations be a useful tool in mineralogy ? This was the topic of a recent CECAM workshop (23-28 June 1997) which was enlivened by a good mixture of experimental

mineralogists, several developers of ab initio codes, and of course a number of practitioners. One theme was mutual education. Up till now one might characterise the community of ab initio computationalists as largely a cosy club of physicists interested in the basics of electronic structure and bonding in condensed matter, knowledgeable about density functional theory, electron correlation, pseudopotentials etc. But here was an embryonic community wanting numbers to such and such accuracy from a black box. Of course they cannot have that, at least not in the foreseeable future, and so what they will need is substantial support. Where is that support to come from, and the interfacing with their complex crystal structure packages etc? It is no answer to say that mineralogists should become physicists; and so we came to the complex issue of commercialisation of codes. Commercialisation of codes has come and will continue, and the question for us is really how to engage with it constructively in a way that also benefits the basic science community. Another point that became evident is that the user community in mineralogy also has specific needs, particularly regarding complicated space group symmetries, large cells with low symmetry, all components of the stress tensor, among others. The mineralogical community is indeed very grateful to the people who have developed various codes, which are drawn on for various purposes, e.g. computation of total energies for processes modelled in large supercells in one case, or the determination of electric field gradients at the nucleus for the interpretation of NMR spectra in another, and so on. One can also make the point the other way round: history has shown in other fields of computational science that codes can get rapidly dropped or superseded if the developers lose touch with the evolving needs of their user community. In addition to the codes being already used in the mineralogical community, the new SIESTA code by Ordejon et al., based on local orbitals which allows calculations of state-of-the-art accuracy at one extreme to very much faster ones of lower accuracy ('quick and dirty') at the other extreme was presented at the workshop and was thought to be potentially very useful for modelling minerals.

Applications in mineralogy can be divided broadly into two streams. One is to design computer experiments to elucidate basic understanding of e.g. phase changes or diffusion processes. We may term this basic mineral physics. For example there are many displacive phase transitions where one may picture the energy as a double well: as the temperature is lowered, the material flops from a more symmetrical structure to the 'left' or 'right' into a less symmetrical structure represented by each of the wells. A puzzle presented at the workshop is that there are marked differences in some cases in the transition along the temperature and the pressure axis: one would like to understand these and the crossover between them.

However more significant for mineralogy and earth sciences generally is simply to get numbers that are difficult, extremely tedious, or impossible to measure in the laboratory. Most obvious are data at the high temperatures and pressures present in the earth's mantle. (A quick teach-in. 'Crust' is the top 30 km of the earth made up of rather low density, complex phases. 'Mantle' is the next 3000 km consisting of a few high density phases where the convection driving the plate tectonics takes place. 'Core' consists of an iron alloy in the middle, liquid and solid respectively in the outer and inner core. The temperature and pressure at the core/mantle boundary are roughly 3500 K and 1.3 Mbar.) Accurate ab initio calculations of elastic constants would

be very valuable in connection with interpreting seismic data, and phonon spectra for thermal enthalpies and entropies. Elastic constants are surprisingly difficult to measure for minerals, partly because there are an awful lot of them, e.g. 21 for a triclinic crystal. A problem of high pressure research is the absence of an absolute pressure scale beyond a few kilobars where one can use a known weight loading with negligible friction. In principle ab initio calculations depending only on the electron mass and charge and other fundamental constant could provide an absolute scale. The challenge was thrown out to calculate either the equation of state of some reference crystal whose lattice constants can be monitored, or the pressure of some phase transition as a marker preferably as a function of temperature. The simulation of materials at high temperature is clearly of great importance (and of difficulty for ab initio calculations!).

Most of what mineralogists would like is way beyond what ab initio calculation can deliver in the near future and a recurring theme in the workshop was to use ab initio calculations to calibrate simulations with empirical interatomic potentials. The latter tend to give good interatomic distances, but the database to which they have been fitted contains virtually no information about relative energies, e.g. about Al in tetrahedral and octahedral coordinations. For example an ab initio calculation of the energy difference between two phases of $ZrSiO_4$ was the first step in a subsequent simulation of radiation damage in a sample with thousands of atoms. The project concerns the use of $ZrSiO_4$ as a host for disposal of plutonium and other actinides.

Almost all naturally occurring minerals are complex solid solutions of two, three or four major components. The synthesis of samples with known composition can be an extremely time consuming and expensive process, but an accurate knowledge of their thermodynamic functions (enthalpy and entropy) is essential for understanding geological processes. There is scope for computer modelling, based perhaps on ab initio calculations on some chosen configurations. Another question is whether one can obtain accurate enough results for solid solutions by defining an average atom, and how would this be done when the components are chemically rather different and have different radii leading to strong strain effects.

Clearly ab initio simulations are not going to solve all the problems of the Earth Sciences but the picture emerged from the workshop that, yes, there are certainly worthwhile research projects for this technique. One young post-doc finds herself besieged by requests for calculations in a department new to ab initio calculations. Another workshop participant spoke of attending an earth sciences conference and seeing a dozen possible projects.

So finally a brief highlight from recent work. Michael Haiber reported an investigation of proton transport in the high pressure phases olivine, forsterite and spinel of Mg_2SiO_4, which may contribute to electrical conduction in the earth's mantle. The three structures are very similar but Mullikan orbital analysis suggested that one of the four oxygen sites in forsterite has a somewhat higher negative charge than the others and indeed a proton gets trapped there with no diffusion observed in ab initio simulations up to 1400 K. However the proton has chains of hydrogen-bond sites with double-well potentials between neighbouring oxygen atoms in one

direction in olivine, and a three-dimensional network of such bonds in spinel. At 1500K there was rapid diffusion in spinel in a two-step process, a jump from one oxygen to the other in the hydrogen bond in about 100 fs and a migration around the oxygen atom to another hydrogen bond in 250 fs. The process has a considerable entropy of activation, a free energy of 0.25 eV being (computationally) measured compared with a barrier energy of 0.17 eV. The electrical conductivity is given by the Einstein relation from the diffusion observed in the simulation. The results show how useful properties of minerals can be obtained at high T and P from ab initio simulation, and how small differences in structure can result in large differences in behaviour.

Vienna–Keele collaboration supported by the Psi-k Network

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Funding from the Psi-k Network has made possible a fruitful collaboration between the groups of Mike Gillan (Keele University, U.K.) and Jürgen Hafner (Technical University, Vienna). The collaboration builds on the shared interests of the two groups in the *ab initio* treatment of liquid and solid metals, but has given benefits which go well beyond this. *Ab initio* techniques developed in Vienna have greatly helped the work of the Keele group on metals, and also in other areas. At the same time, the U.K. experience in parallel implementation of *ab initio* codes has benefited the Vienna group.

Both research groups have a strong background in the *ab initio* theory of metals, using density-functional theory and the pseudopotential approach. At Keele, there has been a major effort over the past four years to apply *ab initio* molecular dynamics simulation to liquid-metal alloys. This research was stimulated by experimental work – particularly by the group of John Enderby at Bristol – on the dramatic variations of structure and electrical properties of liquid alloys with composition. Using the CASTEP code[(1)] written in Cambridge, and its parallel version CETEP[(2)], the Keele group had made fairly extensive investigations of structure and transport properties of the liquid alloys Ga-Se[(3,4)] and Ag-Se[(5–7)] over a wide composition range, working closely with the Enderby group. Because of the need to include d-electrons, the Ag-Se work was computationally demanding, and relied heavily on the Edinburgh Cray T3D. At the same time, the Vienna group had made major advances in technique for treating metallic systems, which were implemented in the VASP code written by Georg Kresse and Jürgen Furthmüller[(8)]. The code has been used for liquid simple metals (Na, Ge)[(8)], liquid transition metals (V,Cu)[(10)], the transition from a liquid metal to an amorphous semiconductor by the rapid quenching of Ge[(11)], and the metal non–metal transition in liquid Hg [(12)].

Because of the common interests, it was clear that collaboration would be extremely beneficial to both groups. To get this moving, Mike Gillan and Janusz Holender (the post-doc working with him on liquid metals) made a three-day visit to Hafner's group in Vienna in November 1995. This visit was made possible by travel and subsistence funding from the Psi-k Network, and brought immediate benefits. Naturally, the two groups got to know each other's scientific work much better. But much more importantly, there was time, even in three days, for detailed discussion of the *ab initio* techniques being used by the two groups. The idea that emerged from these discussions was that the two groups should work together to produce a massively parallel version of the VASP code.

Here, a word is needed about U.K. work on parallel coding of DFT-pseudopotential calculations. Back in 1990, it was realised by Volker Heine, Mike Payne and others in the U.K. that parallel coding was going to play a major role in *ab initio* simulation, and a collaboration was set up to explore this. Initially known as the Grand Challenge consortium, but now called the U.K. Car-Parrinello consortium (UKCP), this collaboration obtained research-council funding to buy a share of a 64-node Meiko Computing Surface at Edinburgh Parallel Computing Centre. This enabled UKCP to build up a major expertise in parallel *ab initio* computations, and CETEP was the DFT-pseudopotential code that emerged from this. The Keele group was a founder-member of UKCP, and made significant contributions to CETEP.

Because VASP has important advantages over CASTEP/CETEP for metals, the potential benefits of parallelising VASP were clear. In making this happen, an important step was a two-week visit of Holender to Vienna in 1996, which was funded by the Psi-k Network. In the end, the comprehensive parallelisation of VASP has been brought to fruition by Georg Kresse, during a 10-month period spent at Keele October 1996 – August 1997. During this period, Kresse has also played a key role in the liquid-metal work of the Keele group, as well as making a number of important technical advances.

Scientific work at Keele for which the collaboration has been crucial includes work on liquid selenium and on liquid and solid iron. Some work on ℓ-Se and ℓ-Te had been done by the two groups before the collaboration was up and running[13], and this had shown that the two systems pose problems for density-functional theory. In the solid, both elements crystallise to form helical chains, with strong covalent bonds within the chains and much weaker bonds between the chains. It is the weak bonds that cause the problem. One sign of this is that the local density approximation (LDA) underestimates the equilibrium lattice parameter for Se perpendicular to the chain axis by about 10 % [14]. Fortunately, this huge error is almost entirely corrected by the generalised gradient approximation (GGA). The LDA also turns out to give pretty mediocre results for the radial distribution function in ℓ-Se (the results are even worse for ℓ-Te). Through the collaboration, we have been able to study this problem in depth for ℓ-Se, and we have shown that GGA produces a big improvement for the liquid as well. This collaborative work led to a joint conference paper [1] which has already been published, and a lengthy paper on ℓ-Se which has been submitted to Phys. Rev. B [2] (reports benefiting from the collaboration are cited in square brackets – see separate list below). A further long paper on defects in ℓ-Se is about to be submitted [3].

In addition to this work on ℓ-Se, the parallel VASP code produced by the collaboration has played a crucial role in our work on liquid and solid iron. Work on iron is being done in both groups, but particularly relevant is a collaborative project between Keele and the group of David Price in London (Geological Sciences Department, University College London). In this project, we are using *ab initio* simulation to help understand the properties of iron in the Earth's core. Specifically, we are using the calculations to shed light on the viscosity of liquid iron in the Earth's outer core, and the pressure-dependent melting point and the phase diagram of solid iron under Earth's-core conditions. Using the VASP code, we have been able to show that DFT-pseudopotential calculations reproduce very well some of the key experimental data on solid and liquid iron at high pressures and temperatures, and we have obtained estimates for the viscosity of the liquid in the outer core. Some of the work has already been reported in a paper

presented at one of the Royal Society of Chemistry's Faraday Discussions [4], and a paper has also been submitted to Nature [5]. In addition, we have used VASP to do *ab initio* calculations on the melting of aluminium, in order to prove the techniques that will be used to study the high-pressure melting of iron, and a paper is in preparation on this [6].

We also want to mention that the parallel VASP code is playing an important part in the work of the Keele group on oxide surfaces, and a joint paper with the Vienna group on this is in course of publication [7]. The work of Georg Kresse at Keele has also led to a number of significant technical advances, including: the parallel *ab initio* implementation of Jonsson's 'nudged elastic band' method for finding transition states; and the implementation of Blöchl's 'projected augmented wave' technique within the VASP code.

In conclusion, we want to thank the Psi-k Network for the travel and subsistence funding which enabled our collaboration to establish itself. The benefits of this funding are already clear from the work reported by the collaboration, and their effect will be felt for many years to come.

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