HCM Newsletter

Ψ_k Network

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

Number 3 June 1994

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Editorial

In this newsletter in the section **News from the Network** we list all research groups from the central and eastern-european countries that have expressed interest in joining our Network.

In the section **News from the Working Groups** you will find reports from some Network related workshops and meetings. There you will also find travel reports of the collaborative visits that have been submitted to us.

Moreover, in this newsletter you will find the final announcement of the Aarhus Workshop including its programme.

In this newsletter there is also an advertisement of a postdoctoral fellowship with professor H. Polatoglou within the HCM programme on *"ENERGY PATHWAYS IN BOND MAKING AND BREAKING AT SURFACES"*.

As usually, you will find the abstracts of the manuscripts recently submitted for publication by members of our Network at the end of the newsletter.

Finally, we would appreciate very much if all your contributions (eg. abstracts, reports) submitted to the forthcoming newsletters were written in the *latex* form. Editing a newsletter is a time consuming task and we would like to minimise the amount of our time spent on converting *ascii* files into the *latex* ones.

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

News from the Network

At the present time our activity concentrates on preparing a proposal to be submitted to Brussels for expanding our Network by including research centres from the central and eastern-european countries. There have been many groups that expressed interest in joining our Network, and we are trying our best to give all of them an equal opportunity. However, it is up to Brussels which and how many of them will be funded. The list of the groups seeking funding follows.

node		e-mail
M. Sob	Brno + Prague (Czech Republic)	mojmir@ipm.cz
A. Kiejna	Wroclaw (Poland)	kiejna@plwruw11.earn
J. Kollar	Budapest (Hungary)	jk@power.szfki.kfki.hu
V. Crisan	Cluj (Romania)	vernes@radix4.mpi-stuttgart.mpg.de
E. Maksimov	Moscow (Russia)	maksimov@td.fian.free.net
V. Antonov	Kiev (Ukraine)	antonov@radix2.mpi-stuttgart.mpg.de
V. Anisimov	Ekaterinburg (Russia)	ifmxr@imm.e-burg.su
N. Kulikov	Moscow (Russia)	hpp@adonis.iasnet.com
A. Lisenko	Kiev (Ukraine)	post@ipms.kiev.ua
A. Matkovskii	Lvov (Ukraine)	saban@sigma.icmp.lviv.ua

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

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

News from the Working Groups

Report on the meeting of the H.f group - Green functions and CPA Muenster, 25th March 1994

The meeting, on the last day of the DPG (German Physical Society) meeting in Muenster, was attended by about 40 people! The following talks were presented, about 20 minutes each:

Zeller: A tight-binding KKR method
Braun: Relativistic photoemission theory applied to GaAs and Os
Schattke: Photoemission and surface screening for semiconductors and layered compounds
Ebert: Activities in Muenchen on relativistic spin-polarized KKR and KKR-CPA
Dederichs: Use of Fermi-Dirac distribution in Green function calculations
Inglesfield: Embedding atoms into a finite-difference grid
Abrikosov: Surface segregation in binary metallic alloys from first-principles calculations
Pollmann and Krueger: Green functions for calculating structural, electronic and vibronic properties of clean and adsorbate-covered surfaces
Crampin: Validity of the 2D scattering approach to laterally confined surface states
Andriotis: Embedding and the complex Hartree-Fock calculational scheme-an interesting comparison

Reports came in from Strange on his work on relativistic spin-polarised KKR-CPA, and from Winter, Szotek and Temmerman on evaluation of correlation functions.

Let's hope that collaborations emerge: we intend to have a similar meeting in a years' time, probably at the end of the next DPG meeting in Berlin.

The abstracts of all presentations and reports follow.

John Inglesfield

A tight-binding KKR method

R. Zeller and P.H. Dederichs
Institut für Festkörperforschung, Forschungszentrum Jülich,
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Abstract

We describe an exact transformation of the conventional KKR method into a tight-binding like form with structure constants which rapidly decay in real space. Our approach differs from previous formulations (see: O.K. Andersen et al., Mat. Res. Soc. Symp. Proc. vol **253**, 37 (1992) and L. Szunyogh et al., Phys. Rev. **B49**, 2721 (1994)) and is based on replacing the usual free-space reference system by one with repulsive constant potentials within the muffin-tin spheres. For periodic crystals the structure constants for this reference system can be calculated by Fourier transformation. Test calculations for an fcc lattice with lattice constant a = 6.76 a.u. and repulsive potentials V =2 Ry yielded structure constants which have decreased already for third-neighbour sites to about 1 percent of the nearest neighbour ones. Because of the rapid decay the structure constants can alternatively be calculated in real space by use of a finite cluster of repulsive muffin-tin potentials. We found that both methods agree very well. The fast decay of the structure constants opens the way to treat surfaces and interfaces as described by Szunyogh et al.

Relativistic photoemission theory applied to GaAs and Os

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Abstract

A fully dynamical one-step model of photoemission for several atoms per unit cell is presented. The theory is a relativistic generalization of the original work due to Pendry and coworkers and allows for calculating ultraviolet photoemission and bremsstrahlung isochromat spectra from pure elemental solids and compounds. Here, the theory is applied to spin-integrated photoemission calculations for the GaAs(110) and Os(0001)-surface. A very good agreement between the calculated spectra and the corresponding experimental data is observed for both systems and all different excitation energies.

Photoemission and surface screening for semiconductors and layered compounds

Wolfgang Schattke
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Abstract

Besides bandstructure calculation and matrix element integration the one-step evaluation of photoemission spectra should at least also consider the electrodynamic properties of the bulk and the surface if not penetrating into the jungle of other vertex corrections. In our investigations we found that the local field effects in the bulk response as well as the surface screening of the external photon field yield a strong influence on the photocurrent. This comes out especially in the anisotropic case of layered crystals and of semiconductor surface states, for which model calculations have been performed. They allowed for a qualitative estimate of the change of the light wave the result being introduced into the one-step calculation. E.g. in the case of TiS_2, including plasmon excitation within a hydrodynamic response model considerably improves agreement with the experimental spectra compared with using Fresnel's formulae of classical textbook optics (Phys. Rev. Letters **68**, 522 (1992)). This applies only for photons above the plasma frequency.

Furthermore a selfconsistent TDLDA-calculation of the surface response for a model solid with surface parallel translational invariance and perpendicular periodic modulation of the ionic background charge density has been carried through to simulate for a system with crystallinity what is known as the surface photoelectric effect in the case of jellium. The agreement with experiment did not change significantly in this photon regime below the plasma frequency, maybe as a consequence of the poor model system. However, a test on the influence of the bulk local fields by merely varying the phase of the dielectric function resulting from this model reflects a strong effect on the spectrum (D. Samuelsen, Ph.D. thesis, Kiel).

For quantitative purposes we determine the full dielectric function for both classes of materials, i.e. including local fields and surface screening in the nonlocal dynamic response function. For the III-V-semiconductors halfspace greensfunctions in a tight binding basis are used which have been determined as a first step halfempirically within the extended Hückel scheme. In the case of layered crystals tight binding wavefunctions have been applied as well, in order to evaluate the microscopic ϵ for the bulk and to get the inversion for the macroscopic dielectric function. In both cases the RPA was used, but in the former localized orbitals and in the latter plane waves determine the final representation.

Spin-polarized relativistic KKR-CPA calculations

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Abstract

Recently we have combined the Coherent Potential Approximation (CPA) approach to deal with disordered alloys with the spin-polarized version of relativistic multiple scattering theory (SPRKKR-CPA). This formalism allows to calculate the electronic structure of magnetic alloys treating all relativistic effects in a rigorous manner. By this way one gets access to a number of interesting spin-orbit induced properties as for example: orbital contributions to the magnetic moments and the hyperfine fields, magnetic X-ray dichroism or magneto-resistivity. Corresponding results are presented for a number of alloy systems as e.g.Fe_xNi_{1-x} and Co_xPt_{1-x} and are compared to experimental data. Some technical aspects of the SPRKKR-CPA-scheme and problems with the LDA, as a framework for these type of calculations, are discussed.

Use of Fermi–Dirac Distribution in Ab-initio Green's Function Calculations

Peter H. Dederichs
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Abstract

We discuss the use of the Fermi–Dirac distribution for finite temperatures in ab–initio ground state calculations based on Green's function methods. The idea is that the smoother cut–off of the occupations at E_F should simplify the numerical procedure. Using the analytical properties of the Fermi–Dirac distribution and the method of complex–energy integration we derive consistent formulas for the charge density and the total energy for finite T. Savings of computer time and higher numerical accuracies can be expected in cases where the $\mathbf{k}$–space integration can only be performed on a point–by–point basis, as e.g. in the special–point method. We illustrate the effect of temperature in calculations for the Ag(001) surface and for magnetic adatoms on this surface.

Surface segregations in binary metallic alloys from first-principles calculations

I.A. Abrikosov[1], A.V. Ruban[2], H.L. Skriver[2], and B. Johansson[1]

[1] Department of Physics, University of Uppsala, Sweden

[2] Center for Atomic-Scale Materials Physics and Department of Physics, Technical University of Denmark, Lyngby, Denmark

Abstract

Local density calculations of surface segregation profiles in random Cu-Ni and Pt-Ni alloys are presented. The theoretical technique is based on the coherent potential approximation and the linear muffin-tin orbitals method. Temperature effects were accounted for by means of the cluster variation method and by mean field theory. The necessary interaction parameters were calculated by the Connolly-Williams method generalized to the case of a surface of a a random alloy.

For the Cu-Ni (001) surface we find the segregation profiles to be oscillatory with a strong preference for Cu to segregate towards the surface for all bulk concentrations and for a wide temperature interval.

For the $Pt_{50}Ni_{50}$ alloy we find that the concentration profiles of the three low index surfaces oscillate and that the two most closely packed surfaces, i.e. (111) and (001) are enriched by Pt while Ni is found to segregate to the surface of the (110) face. These results may be explained in terms of a competition between the tendency of Pt to segregate towards the two first surface layers at the (110) face and the tendency to form a structure of alternating Pt and Ni layers.

Greens functions for calculating structural, electronic and vibronic properties of clean and adsorbate-covered surfaces

Peter Krüger and Johannes Pollmann
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Universität Münster, Germany

Abstract

In this talk both semi-empirical and selfconsistent LDA Greens function calculations for clean and adsorbate- covered surfaces within the scattering theoretic formalism were briefly described.

The first part (given by J. Pollmann) addressed semi-empirical tight-binding calculations for a number of systemsof increasing complexity. As an example of the application of ETBM scattering theory to metal surfaces, the electronic structure of Pb(001), Pb(110) and Pb(111) was presented. Furthermore, the calculation of optimal surface geometries, surface force constants and surface phonons based on a semi-empirical total energy ansatz, using electron and phonon surface Greens functions was discussed. The systems addressed ranged from Si bulk phonons over surface phonons at the Si(001)-(2x1) surface to surface phonons of the H:Si(111)-(1x1) adsorption system. The results for the latter system show excellent agreement with recent HREELS data. Finally, displacement correlation functions for adsorbate-covered surfaces, as calculated using surface phonon Greens functions, were briefly addressed.

In the second part (given by P. Krüger), selfconsistent Greens function calculations for structural and electronic properties of clean and adsorbate-covered (001) surfaces of Si and Ge were addressed. A fair account of some formal and numerical details of the approach was presented. The optimal geometries consisting of asymmetric dimers and the corresponding surface electronic bandstructures of the clean substrates has been discussed. As examples for the adsorption of group V elements on semiconductor surfaces results for As:Si(001)-(2x1), Sb:Si(001)-(2x1) and Sb:Ge(001)-(2x1) have been presented. The physical mechanism for the creation of symmetric adatom dimers observed both in the calculations and in experiment has been explained. The calculated structural properties and the dispersions of the dangling bond and dimer bond bands of these systems is in very good agreement with the results of SEXAFS and ARUPS measurements, respectively. Na:Si(001)-(2x1) has been discussed as a prototype for the adsorption of alkali metals on semiconductor surfaces. For full monolayer coverage, adsorption of sodium at pedestal and valley-bridge sites is observed to be energetically

most favourable. The electronic structure is dominated by hybrid states formed by the Na atoms and the dangling bonds of the Si dimers which still remain in this lattice configuration. The calculated dispersion of the related surface state bands is in excellent agreement with recent ARUPS data. Finally, the work-function lowering by Na adsorption, which is induced by a strong polarization of the adsorbed Na atoms, was discussed.

Influence of bulk states on laterally confined surface state electrons

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M.H. Boon and J.E. Inglesfield
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Abstract

Strong scattering by adatoms positioned with the tip of an STM has recently been used to confine surface state electrons to nanoscale structures. We develop a model for confinement by a circular potential on a metal surface, including substrate band structure effects. Scattering into bulk states provides an important broadening mechanism for partially confined states, and is much more important than partial lateral confinement in determining the level widths. This indicates that more attention should be paid to the choice of substrate than adatom species if the lifetime of the confined electrons is to be maximised, e.g. for nanoscale applications like imaging "scarred" eigenstates in structures corresponding to classically chaotic systems. Contrary to experiment the level width vanishes as the energy approaches the surface state band edge, indicating an additional dominant broadening mechanism for the laterally confined surface state levels seen in the STM.

Embedding muffin-tins into a finite difference grid

J.M. Thijssen and J.E. Inglesfield
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Abstract

A new method is given for calculating the electronic structure of solids, enabling finite difference methods to be applied to general systems. The atoms in the system are surrounded by muffin-tin spheres. The solutions of the atomic-like Schrödinger equation in the muffin-tins are solved using standard numerical techniques and embedded into a finite-difference grid. The interior of each muffin-tin is eliminated from the problem by replacing it by an embedding potential coupling the grid points just outside the sphere. The sparse Hamiltonian matrix of the grid can now be diagonalized, for example using Lanczos techniques, with a computation time linear in the size of the system. Because the Schrödinger equation in the muffin-tins can be solved with arbitrary precision for deep potentials, the method is not restricted to pseudo-potentials, which have to be used when the finite difference grid is extended throughout the system. We present results for fcc copper.

Embedding and the coupled-Hartree-Fock calculational schemes : an interesting combination

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Abstract

The combination of two sophisticated calculational schemes which are used so far independently in Solid State and Atomic/Molecular Physics is proposed as an efficient approach for treating embedded atoms/molecules at a CI level of approximation. In particular, the combination of Inglesfield's embedding method and the Coupled Hartree Fock scheme is proposed.

Preliminary results of such an approach at the non local Hartree- Fock level of approximation are presented and indicate the applicability of the proposed approach to the excited states of the embedded atoms, as for example the embedded Ar(KL3s2 3p5 4s1) atom in jellium.Comparison between the results of the present method and those obtained within the Green's function approach indicates that care should be taken in dealing with the analytic continuation of the complex Hamiltonian of the embedded system.

References

A.N. Andriotis, Europhys. Letters **17**, 349 (1992) and J. Physics: Condensed Matter **4**, L633 (1992).

The Relativistic Spin-Polarized KKR-CPA

A.C. Jenkins and P. Strange
Physics Department, Keele University, Keele, Staffs, ST5 5BG, UK

Abstract

We report recent progress in the development of the KKR-CPA programs used for calculating the electronic structure of random substitutional alloys. A spin-polarized relativistic version of this code has been developed which can be used to treat f-electron alloys. This involves solving 84 simultaneous CPA equations and is very computationally time consuming. Nonetheless some of the most interesting topics in condensed matter physics occur in rare earth and actinide materials. These include valence fluctuations, indirect exchange magnetism and exotic magnetic orderings. Hence we believe that this code can be used to aid our understanding of a variety of problems. The first application of the code has been to the description of $Ce_{0.5}Th_{0.5}$, where we have calculated the electronic structure and predicted the magnetic dichroism spectra at the M_4 and M_5 edges. We would welcome any collaborations with researchers interested in using this code.

The Evaluation of Correlation Functions with the Help of Green's Functions

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Z. Szotek and W.M. Temmerman
DRAL, Daresbury Laboratory, Warrington, WA4 4AD, U.K

Abstract

We have developed an approach to the bandstructure based calculation of the spin-density- and the density-response functions to a level from where it can be applied to systems in the range from nearly free electrons (nfe) to transition metals and ceramics with extremely narrow bands. The ingredients to these kind of calculations, represented by the bandstructure one-particle Green's function, have to be known with high precision for an extended energy range and for all parts of real space including the interstitial regions. Scattering theory satisfies these requirements since in addition it guarantees the fulfillment of various sum rules. Some further development of the approach is needed to apply it to still more complex systems and to implement it with the self-interaction correction (SIC)-augmented bandstructure.

Report on the Workshop of the Working group L: DONTB (Dynamical Order N Tight Binding),

held on 11-12 April 1994 at the Max-Planck-Institut für Metallforschung, Seestrasse 92, D-70174 Stuttgart

LIST OF PARTICIPANTS

(Excluding a number of local participants who came to hear the talks)

Antonis Andriotis, Heraklion, Greece
Alexis Baratoff, Basel, Switzerland
Alex Bradkovsky, Oxford, England
Mike Fearn, Oxford, England
Mike Finnis, Stuttgart, Germany
Chris Goringe, Oxford, England
Peter Gumbsch, Stuttgart, Germany
Olivier Hardouin Duparc, Palaiseau, France
Eduard Hernandez, Keele, England
Wolfgang Hierse, Darmstadt, Germany
Georg Kreuch, Vienna, Austria
Nektarios Lathiotakis, Heraklion, Greece
Tony Paxton, Oxford, England
David Pettifor, Oxford, England
Hariton Polatoglou, Thessaloniki, Greece
Riikka Virkkunen, Helsinki, Finland

PROGRAMME
DONTB (Dynamical Order N Tight Binding) Workshop, 11-12 April 1994

Monday

09.25	**Finnis**	*Introductory Remarks/Discussion of Agenda*
09.30	**Pettifor**	*Recent developments of the bond-order potential*
10.30	**Coffee**	
11.00	**Fearn**	*The Oxford bond-order potential code: application to self-diffusion in Si*
11.45	**Goringe**	*Density matrix methods applied to semiconductor surfaces*

12.30	**Lunch**	
14.30	**Gumbsch**	*Bond-order potentials for transition metals*
15.15	**Bratkovsky**	*HCP Titanium in the tight-binding bond model*
16.00	**Coffee**	
17.15	**Hierse**	*O(N) methods and transferability*
18.00	**Virkunnen**	*Tight-binding interests at the Helsinki Universityr of Technology*

Tuesday

09.00	**Finnis**	*The trouble with metal/ceramic interfaces...*
09.45	**Discussion**	*What do we need: What kind of parameters?*
		New algorithms?
		A common code?
10.30	**Coffee**	

Close of meeting

Additional short talks were given by Tony Paxton (Calculations of the density matrix in Mo) and Hariton Polatoglou (Monte-Carlo calculations of wetting at a grain boundary in Cu3Au).

The workshop brought together a lively mixture consisting of experienced tight-binders, those at the leading edge of the field and those wishing to learn more with a view to future applications. The main discussions of the workshop concerned the relative merits and demerits of two methods of doing O(N) tight-binding with force calculations, namely the bond-order potentials (BOPS) and the variational calculation of a truncated density matrix (RHO). The BOP approach is based on the ideas of Pettifor and coworkers, the latest published formalism being in M.Aoki, Phys.Rev.Lett.23, 3842 (1993). The RHO approach is based on X.-P.Li, R.W.Nunes and D.Vanderbilt, Phys.Rev.B 47, 10891 (1993). The arguments depend very much on whether one is dealing with semiconductors or metals, and localised or delocalised states, as became clear during the workshop.

Tight-binding parameters were not the main topic of discussion, although it was recognised that the new algorithms discussed here can only be as good as the TB parameters which they implement.The challenge here is still to find transferable parameters which reasobably well describe the band structure and elastic properties of the perfect solids.Perhaps this topic should feature prominently in a future workshop?

In their implementation, both BOP and RHO methods have undergone considerable refinement since the last publications.It is not yet clear that one method is superior in all situations. The BOPs have the advantage that they deliver also the Green functions and

response functions, and do not require matrix elements beyond the range of the TB Hamiltonian.Being a moments based method, the BOP does not look so favourable when localised states are present. However, there is still scope for improvement by recurring to inexact levels rather than using a larger cluster. The RHO method has the drawback that the density matrix in metals falls off rather slowly so rather a large variational problem must be solved. On the other hand the density matrix rho from one timestep is a good starting point for iterative refinement at the next timestep in a dynamical simulation, which offers a potential saving as compared to the BOP, in which everything has to be calculated from scratch at each new position of the atoms. In any case it is clear that with more than 100-200 atoms, both O(N) methods are faster than conventional O(N**3) matrix diagonalisation.

The Oxford group emerged as the clear leaders in the development and implementation of both methods.They already have separate codes for each and they are developing a combined code, in which either method may be invoked. This should be the code of choice for any potential users in the network.Anyone wishing to try out the code should discuss a collaborative project with David Pettifor and colleagues in Oxford, so that at least the first paper would be the result of a collaboration. The new user could then work with the code and publish results on their own if they wish. The code under development is designed to run on unix workstations, and no parallel version is on offer at this stage!

The participants generally judged the workshop a success. Antonis Andriotis has already offered to organize the next one in Crete!

Mike Finnis

Report on Collaborative Visit by Mike Finnis

As proposed, I visited the Cavendish Laboratory (Volker Heine) and the Department of Materials in Oxford (David Pettifor, Tony Paxton). I arrived in England on Saturday 30 Oct., spent Monday-Tuesday (2-3/11/93) in Oxford and Wednesday-Thursday in Cambridge.

1. With Volker Heine and Mike Payne we discussed the interpretation of atomistic simulations of Al containing defects. Ab initio calculations and calculations using the Sutton-Chen N-body potential were considered. We concluded that it is necessary to try and match the elastic properties of the empirical potential to those of the ab initio calculation in order to draw conclusions about the role of many body effects or metallic versus pairwise bonding. Also, we concluded that a consistent local definition of the strain needs to be developed in order to visualise the strain distribution during crack extension. I also had long discussions with A.de Vita, with whom we are collaborating in the calculation of the Nb/Al2O3 interface, about the interpretation of our calculations and the role of non-linear core corrections.

2. In Oxford I spent most of the time with Tony Paxton. We installed his LMTO and tight-binding codes on the Silicon Graphics Crimson workstation in Stuttgart. We made a test TB calculation for Al2O3 using his full k-space method and checked that the gamma-point energies agreed with my gamma point program, written independently. We initiated an LMTO calculation for Al2O3.

Mike Finnis
Stuttgart, 9 November 1993

Report by Volker Heine on a visit to Kollekolle/Copenhagen 6-9 January 1994 as part of attendance at Miniworkshop

I had (a) discussions with Martins, Scheffler and Hafner about a summer school type of workshop on dynamics. (b) Scientific discussions with Hafner about dynamics. (c) Discussions with Hafner about a workshop or/and summer school on generating optimised pseudopotentials. (d) Scientific discussions with Jacobsen about their tight binding scheme and our aluminium database. (e) Scientific discussion with Scheffler and Blochl about k-point sampling for metals.

V. Heine

Final announcement, May 11, 1994

Third Aarhus Workshop on

Quantum Theory of Solids:

Improved Density Functionals

Workshop of the Ψ_k Human Capital and Mobilty Network

June 9-10, 1994

Institute of Physics and Astronomy

University of Aarhus

DK 8000 - Aarhus C, Denmark

Thursday, June 9th:

9:00-9:50	**A. Zupan**, Ljubljana,	*Hartree Fock*
9:50-10:40	**F. Aryasetiawan**, Lund,	*GW: Ni and NiO*
11:10-12:00	**F. Manghi**, Modena,	*3-body Scattering Theory*
13:00-13:50	**E. K. U. Gross**, Würzburg,	*Time-dependant DFT*
13:50-14:40	**M. Foulkes**, London,	*Quantum Monte Carlo*
15:10-16:00	**R. Godby**, Cambridge,	*Exact functionals for models*
16:00-16:30	**P. Ziesche**, Dresden,	*Modified HKS Scheme*

Friday, June 10th:

9:00-9:50	**K.-H. Schwarz**, Wien,	*Gradient Corrections*
9:50-10:40	**P. Söderlind**, Uppsala,	*Gradient Corrections*
11:00-11:30	**M. Posternak**, Lausanne,	*Model GW approach to TMO's.*
11:30-12:20	**J. Zaanen**, Leiden,	*LDA+U*
13:20-14:10	**V. Anisimov**, Ekatarinenburg,	*LDA+U*
14:10-15:00	**W. Temmerman**, Daresbury,	*Self-Interaction Corrections*
15:20-16:10	**L. Severin**, Darmstadt,	*Orbital Polarisation Schemes*

Registration is free, and

deadline for registration is May 27th.

Members of the network may apply for money to cover travel and accommodation from the network. In praxis: The accomodation costs will be taken care of jointly for all participants; for other expenses: fill in a travel claims form (obtainable from W. Temmerman or at the meeting).

Accommodation: Hotel Ansgar, Tel.: (+45) 8612 4122
Chairman: Niels Egede Christensen (Aarhus)
Organizer: Axel Svane (Aarhus)
(Tel.: (+45) 8942 3678, Fax: (+45) 8612 0740, e-mail: svane@dfi.aau.dk)

EC POSTDOCTORAL FELLOWSHIP

A twelve-month postdoctoral fellowship is available starting September '94, financed by the EC, within the Human Capital and Mobility programme:

"ENERGY PATHWAYS IN BOND MAKING AND BREAKING AT SURFACES"

in Greece at the Aristotle University of Thessaloniki, to work with ass. prof. Hariton Polatoglou on the above subject using total energy calculations and molecular dynamics.

Applicants must be residents of an EC state, except Greece, and move to Greece during the tenure of the fellowship.

Candidacies, with CV, list of publications and names (and addresses) of two referees should be sent to Hariton Polatoglou, who would be happy to provide full details of the position, at the address:

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Compositional Short-Range Ordering in Metallic Alloys: Band-filling, Charge Transfer, and Size Effects from a First-Principles, All-Electron, Landau-type theory

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Coventry,CV7 4AL, U.K.
D.D. Johnson
Computational Materials Science Department,
Sandia National Laboratories,
Livermore, California, 94551-0969, U.S.A.
F.J. Pinski
Department of Physics, University of Cincinnati,
Cincinnati, Ohio 45221-0011, U.S.A.

Abstract

Using a mean-field statistical description, we derive a general formalism to investigate atomic short-range order in alloys based on a density-functional description of the finite-temperature, grand potential of the random alloy. This 'first-principles', Landau-type approach attempts to treat several contributions (electronic structure, Fermi surface, electrostatics, magnetism, etc.) to the electronic energy on an equal footing. An important ingredient for the statistical averaging is the replacement of the molecular mean fields (Weiss fields) with Onsager cavity fields, which forces the diagonal part of the fluctuation-dissipation theorem to be obeyed. To show its general applicability and usefulness, we apply the theory to three fcc alloy systems. In $Cu_{0.75}Pd_{0.25}$, the incommensurate atomic short-range order is driven by a Fermi-surface effect, in agreement with earlier work. In contrast, $Pd_{0.5}Rh_{0.5}$ exhibits clustering tendencies, with both band-filling and charge-rearrangement effects being important in setting the spinodal temperature at $1150K$, in good agreement with experiment. In the final examples of three nickel-rich NiCr alloys, previously ignored electrostatic effects are found to play a significant role in determining the atomic short-range order.

(submitted to Physical Review B, on 10th January 1994)
LATEX manuscript can be obtained from phrjz@weed.warwick.ac.uk

A 'First Principles' Theory for Magnetic Correlations and Atomic Short-Range Order in Paramagnetic Alloys with Application to $\underline{Cu}Mn$

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Abstract

A formalism is derived for describing both magnetic correlations and atomic short-range order (ASRO) in the paramagnetic state of a magnetic alloy. It is based on a 'first-principles', finite-temperature, electronic density-functional, mean-field Grand Potential of the random alloy in which the thermally induced spin fluctuations are modelled in terms of 'local moments'. For proper comparison, calculations based on this work should be tested against data from experiments on samples at 'high-temperature' (either *in situ* or rapidly quenched). The calculated ASRO can be compared to any atomic diffuse scattering data; whereas, the calculated magnetic correlations must be compared to polarised-neutron diffuse scattering data. We illustrate our theory with an application to a $Mn_{15}Cu_{85}$ alloy, well-known for its spin-glass behaviour at low temperatures. Our results indicate some unusual anti-ferromagnetic correlations, as also found experimentally. We provide a consistent interpretation of the extensive magnetic and atomic neutron scattering data.

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First-Principles, All-Electron Theory of Atomic Short-Range Ordering in Metallic Alloys: $DO_{22}-$ versus $L1_2 - like$ Correlations

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Abstract

We use a 'first-principles' concentration-wave approach based on a finite-temperature, electronic density-functional, mean-field, Grand Potential of the random alloy to investigate the high-temperature atomic short-range order (ASRO) in $Ni_{75}V_{25}$ and $Pd_{75}V_{25}$ solid solutions. Experimentally, these similar alloys both develop $DO_{22} - type$ long-range order at low temperatures but different ASRO at high temperatures. Our calculations describe the measured ASRO well. We compare these results with those found for a hypothetical $Co_{75}Ti_{25}$ solid solution. Since this alloy orders directly from the melt into the $L1_2$ phase, it should exhibit strong $L1_2 - like$ ASRO as we find in our calculations. We analyze the features in the calculated diffuse intensities in terms of various factors in each alloy's electronic structure. Because we have assumed that the atoms are fixed to the Bravais lattice, we discuss two additional examples, $Al_{75}Ti_{25}$ and $Ni_{50}Pt_{50}$, to show the limitations of neglecting atomic displacements. Notably, the Onsager cavity fields that have been incorporated into the theory to conserve the diffuse scattering intensity over the Brillouin zone and to provide a better description of the long-ranged, electrostatic screening effects.

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Three body scattering theory of correlated hole and electron states

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Abstract

We describe a theoretical scheme for the determination of quasi-particle spectra starting from the energy band structure of a metal and treating the on-site Hubbard repulsion beyond the mean-field theory. The method relies upon an expansion of the many-body states in terms of uncorrelated states with a different number of electron hole pairs. By truncating the expansion to include configurations with one or two pairs one can achieve approximate expressions of the electron and hole self-energies. The inter-particle scattering matrices appearing in such expressions are conveniently calculated using the Fadeev approach. Calculations performed for a constant density of states allow to illustrate the role of three-body correlations in the metal-insulator transitions.

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The REVTEX version can be obtained form Manghi@imovx2.unimo.it

THE ENERGETICS AND ELECTRONIC STRUCTURE OF SILVER CHLORIDE

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Abstract

The density-functional pseudopotential method has been used to study the equilibrium lattice parameter, elastic constants, TO frequency, band structure and valence charge distribution of AgCl. The Ag-4*d* electrons are fully included using an optimized pseudopotential. Results for the lattice parameter and the elastic and vibrational quantities are in satisfactory agreement with experiment, as is the calculated valence band width. The relation of the present results with recent Hartree-Fock calculations is discussed.

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The REVTEX version can be obtained from j.m.holender@keele.ac.uk

Calculated electronic structure of the sandwich d^1 metals LaI_2 and CeI_2. Application of new LMTO techniques

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Abstract

The electronic structures of the cubic layered d^1 metals LaI_2 and CeI_2 were calculated using local density-functional theory and the linear muffin-tin orbital method. Special care was taken in the sphere packing used for the atomic spheres approximation. The band structure and the bonding were analysed in terms of projections of the bands onto orthogonal orbitals. The conduction-band structure could be calculated with a down-folded two-orbital basis which then served for the construction of an analytical 2x2 orthogonal, two-center tight-binding Hamiltonian. The conduction band has almost pure Ln-Ln $5d$ e_g character. The x^2-y^2 contribution dominates and is two-dimensional and short ranged. Strong hybridization with the $3z^2-1$ orbital occurs near the saddle point, which is thereby lowered in energy and bifurcated due to the k_z-dispersion provided by the $3z^2-1$ orbital. This strengthens the metal-metal bonds and prevents the nesting instability of the Fermi surface of the half filled x^2-y^2 band. Within the limited accuracy of the LDA, the band structure of CeI_2 was found to be identical to that of LaI_2. The conduction-band $4f$ hybridization $V_{df}^2(0)$ was analysed and found to be several times smaller than in fcc γ-Ce, in qualitative agreement with recent photoemission results. Of importance for this reduction seems to be that the conduction band is formed by essentially only one orbital, Ce $5d_{x^2-y^2}$, that the number of Ce nearest-neighbors is small, and that the Ce-Ce distance is relatively large.

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(Preprints can be obtained from jepsen@radix1.mpi-stuttgart.mpg.de)

Structure and Stability of Ni Clusters: A Tight-Binding Molecular Dynamics Study

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Abstract

The tight-binding molecular dynamics scheme incorporating d-electrons is used to obtain a first systematic set of results for Ni_n clusters in the range $10 < n \leq 55$ by full geometry optimization. The relative stability of fcc structures is compared with the two kinds of icosahedral structures, open and full. Our results show the fcc structure to be more stable than the former, but less stable than the latter in this range. The general trends for Ni_n clusters of this size are well described by our results. The method appears to provide a promising semi-empirical interface in modeling interactions in both covalent and metallic systems.

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Theoretical search for a bistability of apical oxygen in $YBa_2Cu_3O_7$

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Abstract

We report frozen-phonon LDA calculations for $YBa_2Cu_3O_7$ of the infrared- and Raman-acitve apical-oxygen phonons in the c-direction. No sign of the suggested bistability or anharmonicity is found.

(To be published in Philosophical Magazin)
The Revtex copy can be obtained from mazin@radix2.mpi-stuttgart.mpg.de

INFERRED PHYSICAL PROPERTIES OF $\mathbf{UT_2Si_2}$ ($\mathbf{T = Ru, Rh, Pd}$) FROM SPIN-DENSITY FUNCTIONAL CALCULATIONS

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Abstract

The electronic structure of URu_2Si_2, URh_2Si_2 and UPd_2Si_2 is determined by means of selfconsistent density-functional calculations in the local approximation treating the U 5f states as band states. A pronounced trend in the hybridization strength is exposed and is claimed to give rise to the different magnetic properties of these compounds. Thus we found that strong hybridization of the U 5f and Ru 4d states causes URu_2Si_2 to be very close to a nonmagnetic-magnetic instability. The densities of states are calculated and are seen to compare well with results of photoemission experiments.

(sent to Solid State Communications)
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Local Moments of 3d, 4d, and 5d Atoms at Cu and Ag (001) Surfaces

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Abstract

We present ab-initio calculations for the electronic structure of 3d, 4d and 5d transition-metal impurities at the (001) surface of Cu and Ag and determine the surface enhancement of the local moments. For 3d impurities we find a sizable enhancement of the local moments, being most important for V and Cr. Large local moments are obtained for 4d and 5d impurities which are in general non-magnetic in the bulk. Some of the adatoms (Nb, Mo, Tc, W, Re) on Ag (001) have "giant" magnetic moments between 3 and 4 μ_B.

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The REVTEX manuscript can be obtained from karsten@iff174.iff.kfa-juelich.de

Calculation of the residual resistivity and the low-field Hall coefficient of 3d and 4sp impurities in aluminum

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Abstract

We report systematic calculations of the residual resistivity and the low-field Hall coefficient of Al-based dilute alloys with 3d and 4sp impurities, by self-consistently solving the linearized Boltzmann equation. We employ the on-Fermi-sphere approximation, which allows us to combine the full anisotropy of the aluminum Fermi surface, obtained by the four-orthogonal-plane-wave method, with the phase shifts associated with isotropic impurity scattering, evaluated by self-consistent local-density-functional impurity-in-jellium calculations. Our results show that the anisotropic scattering increases the residual resistivity, thus obtaining better agreement with the experiment. Moreover, a consistent interpretation of the observed trends of the low-field Hall coefficient is presented.

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The Revtex copy can be obtained from nstefan@atlas.uoa.ariadne-t.gr

Use of the Lloyd formula for binary alloys

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Abstract

The generalized Lloyd formula and the trace of the Green's function are equivalent expressions for the number of states of electrons in solids. The comparison of these two approaches enables one to estimate the accuracy of the number of states calculations. We study the accuracy of the Lloyd formula and of the trace of the Green's function for the number of states of a binary random alloy in dependence on the cutoff parameter l_{max} in the orbital momentum representation. We show that for transition metals the truncation at $l_{max} = 2$ leads to an essential loss of accuracy. It is necessary to include into consideration the contributions of s, p, d and f-electrons in both approaches to obtain their numerical equivalence. All upper l contributions can be neglected.

We propose a new quadratic extrapolation scheme to solve the coherent potential approximation equation in *one* iteration. We show that the use of the tetrahedron technique for the Brillouin zone integration for calculation of τ-matrix of scattering of an alloy allows to obtain high–precision results with minimum computational efforts. Proposed procedures reduce computational time at least by a factor of 100 in comparison with the standard approaches.

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The REVTeX version can be obtained from hpp@adonis.iasnet.com