

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

Number 4

August 1994

Proposal: ERB4050PL930589

Contract: ERBCHRXCT930369

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Editorial

Apart from the abstracts, in this newsletter you will find **A Postscript to the Dynamical O(N) Tight-Binding Workshop** by M. Finnis, and some reports from recent workshops and collaborative visits. Moreover, we have an announcement of a post doctoral fellowship. With respect to collaborative visits we need to get your reports as soon as possible. We have to keep track of all the visits and we would also like to publish those reports in our newsletter for every member's information. Please, prepare the reports in latex/revtex form.

Recently, some of you have complained about the length and the amount of information contained in our newsletter. Apparently, many of you have no time to read through it completely. There have been suggestions to limit the size of abstracts to one or two sentences. Therefore, we would appreciate if you could tell us what you think about that and what you expect from the newsletter.

We would appreciate very much if the abstracts submitted to our **Abstracts Information Section** were emailed exclusively to **psik-coord@daresbury.ac.uk** and were **no longer** than one page. The following set of LATEX commands would be preferable in constructing abstracts:

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\newpage
\null
\vskip 2em
\begin{center}
{\LARGE title\par}
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  authors \\
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(submitted to name of the journal) \\
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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

Dzidka Szotek & Walter Temmerman

News from the Working Groups

A Postscript to the Dynamical $O(N)$ Tight-Binding Workshop: Whither Tight-Binding?

Our DONTB workshop in April was necessarily restricted in scope. We covered some exciting developments in $O(N)$ methods, however, as Antonis Andriotis From Heraklion pointed out at the time, the vital issue of how to get reliable TB parameters was not addressed. This and the issue of non-orthogonal basis are an active research topic of the Heraklion group, in collaboration with K.R. Subbaswamy, John Connolly and Madhu Menon(email: super250@ukcc.uky.edu) of the Universty of Kentucky. At the workshop, we heard about the cluster calculations for Ni from Andriotis and Lathiotakis, who showed how Ni only prefers its bulk fcc structure in clusters of more than several tens of atoms. Clusters smaller than about 100 atoms prefer to adopt an icosohedral structure. This week, the Stuttgart group has enjoyed a visit from Madhu Menon who told us more about the activities on the Greece-Kentucky axis, which deserve wider publicity.

Their approach is non-orthogonal empirical TB, with an overlap (S) matrix assumed proportional to H. The parameters are fitted to valence band structure except for three, which are fitted to the bond length and vibration frequency for the dimer (or lattice parameter and bulk modulus for the bulk). The fit is not unique. The usual repulsive potential of TB theory turns out to be very small - it has been largely replaced by the explicit non-orthogonality. The parameters are assumed to decay exponentially, with no special cut-off functions.

The claim (and a challenge) is that the non-orthogonality makes the parameters much more transferable than those of an orthogonal TB scheme. Calculations have focussed on clusters of C, Si and SiC, besides $Ti_n C_m$ and Ni. For the transition metals, d and s orbitals were included. Typically, vibration frequencies of clusters could be obtained with errors of order 20% compared to 100% errors with orthogonal TB. For Si and C in bulk, the diamond structure was found to have lowest energy, whereas clathrate structures have a lower energy than diamond if orthogonal TB is used. An interesting case study was Si_9 , for which they found a new low symmetry structure, subsequently confirmed by LDA and Hartree-Fock calculations to have a lower energy than any structures previously considered. For C clusters, linear, planar and cage structures were investigated. The ring structures showed Jahn-Teller distortions in agreement with ab-initio predictions. These distortions are not predicted by orthogonal TB.

The work of Sankey and Drabold at Arizona, and P.Ordejon at the University of Illinois, also using non-orthogonal TB of a more ab initio kind, seems to support these conclusions. So what are the limits of orthogonal versus non-orthogonal TB? Food for the next workshop?

References

M.Menon, J.Connolly, N.Lathiotakis and A.Andriotis, Phys. Rev. B. in press.

N.Lathiotakis, A. Andriotis, M.Menon and J.Connolly, Europhysics Letters, submitted.

P.Ordejon, D.Lebedenko and M.Menon, Phys.Rev.B in press.

M.Menon and K.R.Subbaswamy, Phys.Rev.B, **47**, 12754, (1993).

M.Menon, K.R.Subbaswamy and M.Sawtarie, Phys.Rev.B **48**, 8398, (1993).

Mike Finnis
Stuttgart 7.7.94

Report on the Workshop on ELECTRONS IN DIFFERENT DIMENSIONS, May 8-14, Varenna, Villa Monastero, Italy

List of Participants

J.G.Aguilar, Santander, Spain; G.Bachelet, Roma, Italy; L.C.Balbas, Valladolid, Spain; O.Bisi, Trento, Italy; C.Br chignac, Orsay, France; M.Broyer, Villeurbanne, France; P.Cahuzac, Orsay, France; H.Haberland, Freiburg, Germany; R.Ferrari, Trento, Italy; J.Fink, Dresden, Germany; N.Van Giai, Orsay, France; C.Guet, Grenoble, France; Ellart, Freiburg, Germany; A.Liebsch, Juelich, Germany; P.E.Lindelof, Copenhagen, Denmark; E.Lipparini, Trento, Italy; H.Lueth, Juelich, Germany; M.Manninen, Copenhagen, Denmark; M.Pellarin, Lyon, France; G.Papadogonas, Crete, Greece; H.M.Polatoglou, Thessaloniki, Greece; F.Rapisarda, Trieste, Italy; Schmidt, Freiburg, Germany; G.Senatore, Trieste, Italy; S.Stringari, Trento, Italy; Ll.Serra, Mallorca; F.Toigo, Padova, Italy; A.Vitturi, Padova, Italy

Program

Monday 9

- Senatore: *Density-density static response of the 2- and 3-D electrons (I): a diffusion Monte Carlo evaluation*
- Fink: *Plasmons in Solids I*
- Ferrari: *Brief review of Quantum Hall Effect*
- Haberland: *Optical response of cold and hot sodium clusters*
- Lueth: *Quantum wires: preparation and transport*
- Manninen: *Electron gas clusters: the ultimate jellium model*

Tuesday 10

- Senatore: *Density-density static response of the 2- and 3-D electrons (II): usage in density functional schemes*
- Lueth: *Porous silicon: a quantum-wire like system*
- Ferrari: *Hartree-Fock approach to Quantum Hall Effect*
- Toigo: *Structural, electronic and magnetic properties of Rh clusters*
- Liebsch: *Influence of bound d states on the dispersion of surface plasmons and of Mie resonances*
- Fink: *Plasmons in Solids II*

Wednesday 11

- Bisi: *Introduction to porous silicon*
- Bachelet: *Absorption peaks, sum rules and the electron-ion interaction in atoms, clusters and solid metals*
- Serra: *Microscopic effective interaction between electrons: applications to metal clusters*

Thursday 12

- Bisi: *Auger lineshape analysis of porous silicon: theory and experiment*
 - Polatoglou: *Optical properties of the ultrathin Si/Ge superlattices and Si wires*
 - Aguilar: *Vibrational properties of sodium clusters*
 - Brechignac: *Collective excitations in clusters*
- 16.45 Coffee break
- Broyer: *Electronic structure of trivalent metal clusters - Influence of the temperature*

Friday 13

- Lindelof: *Level statistics from conductance measurements on quantum dots*
 - Stringari: *Edge waves in the Quantum Hall Effect*
- 10.30 Coffee break
- Guet: *Ground-state correlations in metallic clusters. The RPAE and the MBPT approaches*

The workshop has been focused on the dynamical properties of systems of electrons in different dimensions from both experimental and theoretical points of view, in both infinite and finite systems. The common interest, electrons in different dimensions, covers very different fields, like clusters, quantum wells, wires and dots. Therefore the meeting was not focused on specific arguments or techniques; the main result was to provide a valuable opportunity for the exchange of information among researches working in different areas. The new collaborations established among the participants is a measure of the success of this workshop.

(O. Bisi)

Report on *HCM-ELECTRONIC STRUCTURE NETWORK*
"MAGNETIC SURFACES, INTERFACES AND
MULTILAYERS"
VIENNA 1994

Organizers: P. H. Dederichs and P. Weinberger

Local committee: V. Drchal, J. Kudrnovsky, J. Redinger and L. Szunyogh

PROGRAM

Sunday, May 29th 1994

08:45 - 09:00		Opening remarks, technical details
	<i>Chairman: P. Weinberger</i>	
09:00 - 09:40	B. L. Gyorffy:	"Multilayers and Interface Coupling"
10:00 - 10:40	P. H. Dederichs:	"Interlayer Coupling and Quantum Well States in Co/Cu Bilayers"
11:00 - 11:40	J. Kübler:	"Non-collinear Coupling in Multilayers"
12:00 - 12:40	H. Ebert:	"Dichroism in Multilayers"
13:00 - 14:00		Lunch Break
	<i>Chairman: B. L. Gyorffy</i>	
14:00 - 14:40	P. Bruno:	"Novel results in the theory of interlayer coupling"
15:00 - 15:40	V. Drchal:	"Magnetic Coupling of Interfaces"
16:00 - 16:40	F. Gautier:	"Multilayer and Interface Coupling"
17:00 - 17:40	M. Richter:	"Magnetic properties and Fermi surfaces of multilayers"

Monday, May 30th 1994

Chairman: F. Gautier

- 09:00 - 09:40 L. Szunyogh: "The spin-polarized relativistic screened KKR-method for semi-infinite systems and its applications"
- 10:00 - 10:40 B. Johansson: "Surface Magnetism and Interlayer Coupling"
- 11:00 - 11:40 S. Blügel: "Magnetic Surface Alloys"
- 12:00 - 12:40 I. Turek: "Magnetic properties of surfaces of alloys"
- 13:00 - 14:00 Lunch Break

Chairman: P. H. Dederichs

- 14:00 - 14:40 R. Zeller: "Magnetic impurities at surfaces"
- 15:00 - 15:40 H. Dreyse: "Magnetic ultrathin films"
- 16:00 - 16:40 J. Redinger: "Magnetic surface and interface states"
- 17:00 - 17:40 J. Hafner: "Non-collinear spin-structure in amorphous magnets and magnetic layers"

Tuesday, May 31th 1994

Chairman: B. Johansson

- 09:00 - 09:40 I. Mertig: "Interlayer coupling across $\text{Cu}_x\text{Au}_{1-x}$ spacers"
- 10:00 - 10:40 J. Staunton: "Atomic short range and magnetism in alloys"
- 11:00 - 11:40 J. Kudrnovsky: "Finite critical temperatures of two-dimensional magnets"
- 12:00 - 12:40 W. M. Temmerman: "SIC and Magnetism"
- 13:00 W. M. Temmerman: "Closing remarks on behalf of the HCM"

REPORT ON THE WORKSHOP

The workshop took place at the Institute of Technical Electrochemistry of the Technical University Vienna. It was attended by 28 participants (see the list below). After each talk there was ample time for discussions and the whole atmosphere was very relaxed and friendly. Especially welcome was the participation of the Czech and Hungarian researchers which had very nice contributions. More than 50% of the total expenses were covered by the Austrian group, mostly with money from the Austrian HCM funds. Only the travel expenses of the

"western" participants, amounting to about 4000 ECU, were paid by the network. The local organisation worked very well and we should thank Peter Weinberger and his team for all the efforts and the most generous funding. All people agreed that it was a successful meeting.

Except for the multilayer conference in Düsseldorf, our next network meeting will be next year. Since Balazs Gyorffy will be organizing the Europhysics Research Conference on "Magnetism", we agreed to attach a 1- to 1 1/2-day symposium on "Surface and Interface Magnetism" to this meeting with (mostly) contributed papers.

(P. H. Dederichs)

PARTICIPANTS

- C. Blaas**, Institut für Technische Elektrochemie, TU Vienna, Austria
- S. Blügel**, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany
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- P. H. Dederichs**, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany
- V. Drchal**, Institute of Physics, Czech Academy of Science, Praha, Czech Republic
- H. Dreyssé**, Institut de Physique et Chimie des Materiaux de Strasbourg, France
- H. Ebert**, Institut für Physikalische Chemie, München, Germany
- F. Gautier**, Institut de Physique et Chimie des Materiaux de Strasbourg, France
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P. Weinberger, Institut für Technische Elektrochemie, TU Vienna, Austria
R. Zeller, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

BUDGET

	ECU	Schilling
Austrian HCM-Contribution (PW node)		47 550
HCM-Network Contribution	4000	
Joint Austro-Hungarian-Czech Project		8 100

**Report on the collaborative visit
of C. Patterson (Dublin) to J. Inglesfield (Nijmegen) 24-25
January, 1994**

The visit enabled CP and JI and his group to discuss (i) calculations of bond polarisabilities for optical property calculations and (ii) using Green's Function (GF) techniques to embed clusters with configuration interaction (CI) wave functions.

(1) Both research groups have been using bond polarisabilities to calculate optical properties of semiconductors. They presently use different techniques and discussed them during the visit. The groups have decided to collaborate in this area. Since the visit the discussion has prompted CP to think further on the method of calculating bond polarisabilities and to establish a link between the "electronic phonon" model for optical susceptibilities and the usual optical susceptibility model (direct transitions).

(2) Embedding clusters with CI wave functions using GF techniques is desirable for computing ground state properties of some 'difficult' systems since electron correlation can be included in the cluster part. Excited states involving single particle excitations can probably not be treated adequately by this method and the groups do not presently have any plans to collaborate here.

I think John and I will be collaborating in future. The two areas - bond polarisability and embedded wave functions may merge at some stage. What we are presently doing is Lorentz models for optical properties and comparing these to time-dependent HF. We may do embedded self-energy calculations using a HF starting point and clusters rather than LDA and periodic boundary conditions. Are there any people on the network who are doing GW or other self-energy type calculations?

(C. Patterson)

**Report on the collaborative visit
of Jose Luis Martins to Antwerpen**

A collaboration was started with the visit of J. L. Martins (Lisboa) to P. Van Camp and V. Van Doren (Antwerpen) to study semiconductor materials. An abstract on the phase transformation of AlAs has already been submitted to a conference, and plans for future collaboration on nitride materials established.

(Jose Luis Martins)

**Report on the collaborative visit
of Z. Szotek and W. M. Temmerman at the Laboratoire de
Chimie Physique-Matiere et Rayonnement,
Universite Pierre et Marie Curie in Paris, on March 2–6, 1994**

The purpose of our visit to Paris was twofold. Firstly, we had to finalise arrangements concerning the last NMB meeting (3 March, see number 2 of the Network's newsletter). Secondly, we performed calculations and had extensive discussions with J. M. Mariott and Coryn Hague (belonging to node Boureau) on vanadium oxides and their spectroscopic data. The key issues are the localisation of the vanadium *d* states and the hybridisation of the metal *d* states with the O *p* states. In a systematic study of the *XAS* and *XES* Mariott and Hague are just addressing these issues. The aim of this collaboration is to develop, in parallel, a systematic theoretical picture and in comparison with those experimental studies to develop our knowledge about these materials. The LSD calculations, using the standard LMTO code, for VO, V₂O₃, VO₂ and V₂O₅ lead to an electronic structure of strongly hybridised vanadium *d* bands and oxygen *p* bands. In case of V₂O₃, VO₂ and V₂O₅ the hybridised O *p* band is centered about 4 eV below Fermi energy E_f , in good agreement with experiment, but the binding energy of oxygen 2*s* state is 4.5 eV too small. A quite different result is obtained for VO, where the binding energy of the oxygen 2*s* state is approximately as expected, but the oxygen *p* band is calculated to lie about 4 eV too high in binding energy (this anomaly follows closely the result by Neckel et al. (J. Phys. C **9** (1976) 579) using the LCAO approach). Therefore, we have performed some more LSD and self-interaction corrected (SIC)-LSD calculations for VO and VO₂ systems using our downfolded LMTO code, allowing to correctly account for the tails of the higher partial waves both in the lower, O 2*s*, energy panel as well as in the upper, valence band, energy panel. This allows to study the sensitivity of the results to different procedures in the choice of the basis functions. Moreover, the hope was that a better agreement between the calculated and measured data could be obtained in case of SIC-LSD calculations. That expectation was based on our (Z. Szotek, W.M. Temmerman and H. Winter, Phys. Rev. B **47** (1993) 4029) and Svane and Gunnarsson's (Phys. Rev. Lett. **68** (1990) 1148) results for other transition metal oxides. Our collaboration on VO is being continued.

Z. (Dzidka) Szotek

ANNOUNCEMENT

POST DOCTORAL FELLOWSHIP FOR FIRST PRINCIPLES TOTAL ENERGY CALCULATIONS OF THE ELECTRONIC PROPERTIES OF HEAVY FERMION COMPOUNDS

An Engineering and Physical Sciences Research Council funded position will become available after 1 January to work in collaboration with G A Gehring at Sheffield and W M Temmerman and G Y Guo at Daresbury Laboratory on the theory of Heavy Fermion Compounds of particular interest to the UK experimental programme. The work will include an investigation of the nature of the exotic ground states which may be insulating, magnetic or metallic and will include detailed comparison with experimental data on the Fermi surface. Further details may be obtained from G.Gehring@sheffield.ac.uk or W.M.Temmerman@dl.ac.uk. Applications for the post, including the names of two referees, should be made to G A Gehring at the Physics Department, University of Sheffield, Sheffield S3 7RH or by e-mail.

Surface energy and work function of the light actinides

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Abstract

We have calculated the surface energy and work function of the light actinides Fr, Ra, Ac, Th, Pa, U, Np, and Pu by means of a Green's-function technique based on the linear muffin-tin orbitals method within the tight-binding representation. In these calculations we apply a recent energy functional which combine the kinetic energy calculated within the atomic sphere approximation with Coulomb and exchange-correlation energy terms calculated by means of the complete non-spherically symmetric charge density derived from the atomic-sphere potential within non-overlapping and space-filling cells. The calculated surface energies and work functions are in good agreement with the limited experimental data.

(to appear in Phys. Rev. B **49** in May, 1994)

The REVTEX manuscript can be obtained from jk@power.szfki.kfki.hu

Full Charge-Density Calculation of the Surface Energy of Metals

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Abstract

We have calculated the surface energy and the work function of the $4d$ metals by means of an energy functional based on a self-consistent, spherically symmetric atomic-sphere potential. In this approach the kinetic energy is calculated completely within the atomic sphere approximation (ASA) by means of a spherically symmetrized charge density while the Coulomb and exchange-correlation contributions are calculated by means of the complete, non-spherically symmetric charge density within non-overlapping, space-filling Wigner-Seitz cells. The functional is used to assess the convergence and the accuracy of the linear muffin-tin orbitals (LMTO) method and the ASA in surface calculations. We find that the full charge-density functional improves the agreement with recent full-potential LMTO calculations to a level where the average deviation in surface energy over the $4d$ series is down to 10 %.

(to appear in Phys. Rev. B **49** in June, 1994)

The REVTEX manuscript can be obtained from jk@power.szfki.kfki.hu

Self-consistent Localized KKR Scheme for Surfaces and Interfaces

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Abstract

A Greens function technique is presented that describes the electronic properties of surfaces and interfaces in the framework of multiple scattering theory as based on localized structure constants. Results of self-consistent calculations are presented for the Cu (111), (110) and (100) surfaces. The obtained surface densities of states and work functions are in good agreement with previous calculations.

(appeared in Phys. Rev. B **49**, 2721, 1994)

The Selfconsistent Fully Relativistic Screened KKR Green's Function Method. Applications to the (100), (110), and (111) Surfaces of Au and Pt

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Abstract

The fully relativistic version of the Screened Korringa–Kohn–Rostoker (SKKR) method is discussed and applied charge selfconsistently to the (100), (110), and (111) surfaces of Au and Pt. In comparison to corresponding semi-relativistic calculations for Au it is found that spectral densities very crucially depend on the inclusion of relativistic effects. In terms of work functions, however, the difference between the semi-relativistic and the relativistic calculations is rather small.

(to appear in J. Phys. Condensed Matter, 1994)

The REVTEX manuscript can be obtained from bu@power.szfki.kfki.hu

Normconserving and ultrasoft pseudopotentials for first-row and transition elements

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A–1040 Wien, Austria

Abstract

The construction of accurate pseudopotentials with good convergence properties for the first-row and transition elements is discussed. We show that by combining an improved description of the pseudowavefunction inside the cut-off radius with the concept of ultrasoft pseudopotentials introduced by Vanderbilt (1990 *Phys. Rev. B* **41**, 7892) optimal compromise between transferability and plane-wave convergence can be achieved. With the new pseudopotentials basis-sets with no more than 75–100 plane-waves are sufficient to reproduce the results obtained with the most accurate normconserving pseudopotentials.

(submitted to J. Phys. CM)

Preprint available from jhafner@email.ac.at

Theory of the crystal structures of selenium and
tellurium:
The effect of generalized–gradient corrections to the
LDA

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Abstract

The crystal structure and phase stability of Selenium and Tellurium have been investigated by total energy calculations within the local density approximation, without and including generalized gradient corrections. We find that the LDA underestimates the equilibrium volume by as much as 15 percent and predicts a crystal structure that is much more isotropic than observed: the nearest neighbour distances in the helical chains are increased, but the interchain distances are reduced. Adding generalized–gradient corrections (GGC) to the LDA results in a crystal structure, equilibrium volume and binding energy in better agreement with experiment. We show that the effect of the GGC’s is to add a uniform internal pressure to the system, the local bonding properties at constant volume however are unchanged.

(submitted to Phys. Rev. B)

Preprint available from jhafner@email.tuwien.ac.at

Structural, electronic, and magnetic properties of Fe–Y alloys

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A–1040 Wien, Austria

Abstract

Results of *ab-initio* calculations of the structural, electronic, and magnetic properties of crystalline and amorphous Fe–Y alloys are presented. The structure of the amorphous phases is generated via a simulated molecular–dynamics quench, based on effective interatomic forces derived from tight–binding–bond theory. The results show that a pronounced chemical short–range order (preferred heterocoordination) exists at all compositions and that at short distances the local topology is similar in the crystalline and glassy phases. In the Y–rich alloys, medium–range concentration–fluctuations are superposed to the local order. The investigation of the electronic structure using self–consistent spin–polarized linear muffin–tin orbital (LMTO) calculations confirms that the bonding properties are similar in the crystalline and amorphous phases. The crystalline compounds are ferrimagnetic, the negative Y–moment is induced by a strong covalent interaction of the Y–d band with the minority–spin Fe–d band. Ferrimagnetism is also found in the amorphous alloys. In the Fe–rich range (more than 80 at–% Fe) competing ferro– and antiferromagnetic Fe–Fe exchange interactions lead to coexisting positive and negative Fe–moments. The decrease of the magnetic moments of the Fe–atoms with increasing Y–content is strongly influenced by the strong coupling of the Fe–spins to the Y–moments — as a consequence a spontaneous Fe–moment exists even at very small Fe–Fe coordination numbers. In addition the structural inhomogeneity of the Y–rich amorphous alloys leads to cluster–magnetism.

(to appear in Phys. Rev. B)

Preprint available from jhafner@email.tuwien.ac.at

Ab-initio molecular dynamics simulation of the liquid-metal to amorphous-semiconductor transition in Germanium

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A-1040 Wien, Austria

Abstract

We present ab-initio quantum-mechanical molecular-dynamics simulations of the liquid-metal to amorphous-semiconductor transition in Ge. Our simulations are based on: (a) finite-temperature density-functional theory of the one-electron states, (b) exact energy-minimization and hence calculation of the exact Hellmann-Feynman forces after each molecular-dynamics step using preconditioned conjugate gradient techniques, (c) accurate nonlocal pseudopotentials, and (d) Nosé-dynamics for generating a canonical ensemble. This method gives perfect control of the adiabaticity of the electron-ion ensemble and allows to perform simulations over more than 30 picoseconds.

The computer-generated ensemble describes the structural, dynamic, and electronic properties of liquid and amorphous Ge in very good agreement with experiment. The simulation allows to study in detail the changes in the structure-property relationship through the metal-semiconductor transition. We report a detailed analysis of the local structural properties and their changes by an annealing process. The geometrical, bonding and spectral properties of defects in the disordered tetrahedral network are investigated and compared with experiment.

(to appear in Phys. Rev. B)

Preprint available from jhafner@email.tuwien.ac.at

Electronic structure of approximant phase to icosahedral Ti-transition-metal quasicrystals

M Krajčí and J Hafner

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Abstract

We report ab-initio calculations of the electronic structure of large-unit-cell approximant phases to icosahedral Ti- transition-metal quasicrystals and of disordered alloys of the same composition. Our results demonstrate that the approximant phase is stabilized relative to the body- centred solid solution by the formation of a broad pseudogap at the Fermi-level. The conditions for the formation of the pseudogap are discussed in relation to the atomic structure.

(accepted by Europhys. Lett.)

Preprint available from jhafner@email.tuwien.ac.at

A study of approximations made evaluating the residual electrical dc resistivity of disordered alloys

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Abstract

The residual electrical dc resistivity of the transition metal alloy system Cu–Pt is evaluated by making use of the relativistic version of the KKR–CPA and the one-electron Kubo–Greenwood formula for disordered systems. Starting from the results of a previous calculation the influence of truncation of the angular momentum expansion, the effects of self-consistency of the alloy potential, the importance of vertex-corrections and the difference between the non-relativistic and the relativistic current operator are examined.

(submitted to PRB)

REVTEX-file available from he@gaia.phys.chemie.uni-muenchen.de

First-principles investigations of atomic disorder effects on magnetic and structural instabilities in transition metal alloys

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Abstract

In this paper we use the CPA within the KKR bandstructure scheme to investigate the influence of atomic disorder on magnetism and crystal structure in transition metal alloys like iron-nickel. This method allows an investigation of disordered alloys on an equally well defined basis as an investigation of corresponding stoichiometrically ordered phases. In particular we have calculated the binding surfaces of fcc $\text{Fe}_x\text{Ni}_{1-x}$ for concentrations close to the critical concentration $x = 0.65$ which corresponds to the Invar alloy $\text{Fe}_{0.65}\text{Ni}_{0.35}$, with the help of the Fixed-Spin-Moment method. We find that magnetism in the ground state gradually vanishes as we go from $\text{Fe}_{0.6}\text{Ni}_{0.4}$ which has a well defined magnetic ground state being separated from the nonmagnetic state by 1.0 mRy/atom, to $\text{Fe}_{0.75}\text{Ni}_{0.25}$ which is nonmagnetic. The critical concentration for which this disorder driven magnetic-nonmagnetic transition occurs is $x \approx 0.65 - 0.70$ in accordance with the magnetic phase diagram of $\text{Fe}_x\text{Ni}_{1-x}$. These calculations have to be compared with ab initio calculations for ordered fcc $\text{Fe}_{0.75}\text{Ni}_{0.25}$; here the magnetic ground state is by 1.25 mRy more stable than the nonmagnetic state. This different magnetic behaviour of disordered and ordered phases can be explained on statistical grounds. Furthermore, the nonmagnetic disordered ground state is unstable with respect to a martensitic fcc \rightarrow bcc transition for $x > 0.65$ in accordance with the structural phase diagram of $\text{Fe}_{1-x}\text{Ni}_x$. We have furthermore calculated the temperature evolution of the binding surfaces with the help of a finite-temperature fluctuation theory. We find interesting reentrant ferromagnetic phase transitions in the fcc phase close to the Invar concentration $x = 0.65$.

(submitted to PRB)

REVTEX-file available from he@gaia.phys.chemie.uni-muenchen.de)

Calculation of magnetic X-ray dichroism (MXD) spectra
using the spin polarized relativistic
linear-muffin-tin-orbital
method of band structure calculation

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Abstract

The description of the electronic structure of magnetic transition metal systems by using the spin polarized relativistic linear-muffin-tin-orbital (SPRLMTO) method of band structure calculation leads to a very efficient and reliable way to calculate their magnetic X-ray dichroism (MXD) spectra. This is demonstrated by comparing results for the $L_{2,3}$ -spectra of pure Fe with spectra obtained using the numerically more accurate but computationally more demanding spin polarized relativistic Korringa-Kohn-Rostoker (SPRKKR) method.

(submitted to SSC)

Postscript-file available from he@gaia.phys.chemie.uni-muenchen.de

SPIN FLUCTUATIONS IN γ -Fe AND IN Fe₃Pt INVAR FROM LOCAL-DENSITY-FUNCTIONAL CALCULATIONS

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Abstract

The electronic structure and the ensuing magnetic properties of γ -Fe and Fe₃Pt Invar are determined using the local approximation to spin-density functional theory and the ASW method. A noncollinear constrained-moment procedure is described and employed to obtain the total energy as a function of the volume and the magnetic moment arranged both in collinear and noncollinear spiral structures. This on a microscopic basis establishes the connection of the volume with longitudinal and transverse spin fluctuations. We determine the thermal expansion coefficients of γ -Fe and Fe₃Pt and give an explanation of their anomalous magnetovolume properties.

(to appear in Phys. Rev. B)

Manuscript can be obtained from: kubler@mad1.fkp.physik.th-darmstadt.de (J. Kübler)

First-principles calculation of magnetic x-ray dichroism in Fe and Co multilayers

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Abstract

A relativistic, spin-polarized band theory of magnetic x-ray dichroism (MXD) in solids is briefly described. Calculated circular and linear dichroic x-ray absorptions at the $L_{2,3}$ edges from bulk Fe and Co as well as from their multilayers (Fe_2Cu_6 (001), Fe_1Ag_5 (001), $\text{Co}_2\text{Pd}(\text{Pt})_4$ (111) and Co_2Cu_6 (001)) are presented. Large circular MXD is predicted in both the bulks and the multilayers whilst linear MXD due to magnetocrystalline anisotropy is found to be small (within 1 %). Nevertheless, linear MXD due to a photon polarization change is about 3-8 %. The orbital magnetization sum rule of B. T. Thole, et al. [Phys. Rev. Lett. **68**, 1943 (1992)] is found to give orbital magnetic moments too small by about 20-35 %. We note that for each ion species, there is a simple linear relationship between the integrated circular MXD signal and the orbital magnetic moment, and we propose that one uses this linear relationship to measure the orbital magnetic moment of an ion in magnetic solids. The recently proposed spin magnetization sum rule [P. Carra et al. Phys. Rev. Lett., **694** (1993)] is found to give rather accurate spin magnetic moments for the Co systems (errors within 15 %). However, it does not hold qualitatively for highly anisotropic systems such as Fe multilayers.

(Phys. Rev. B, 1994 (in press))

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Relativistic photoemission theory for space-filling potentials

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Abstract

In this contribution we present as a direct generalization of the recently developed full-potential photoemission theory a relativistic theory for space-filling cell potentials. This theory is based on the well-known one-step model of photoemission. The Dirac equation is solved for space-filling cell potentials, using the relativistic phase functional approach. A practical scheme to calculate the generalized spin-density matrix of the photocurrent is described. The relationship between the new model and the widely used relativistic muffin-tin like theory, as well as the connection to non-relativistic full-potential photoemission is discussed. Moreover, a detailed analysis of the angular matrix elements and the selection rules for a single cell potential in the relativistic and non-relativistic case is given.

(submitted to Phys. Rev. B)

RevTeX manuscript can be obtained from: mgrass@dosuni1.rz.Uni-Osnabrueck.DE

Structure and Phase Stability of $\text{Ga}_x\text{In}_{1-x}\text{P}$ Solid Solutions from Computational Alchemy

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Abstract

The structural and thermodynamical properties of $\text{Ga}_x\text{In}_{1-x}\text{P}$ solid solutions are studied using Monte Carlo simulations based on density-functional perturbation theory. The free-standing alloy displays a model random behavior, with a miscibility gap below ~ 820 K. In samples grown on a GaAs (001) substrate, the resulting epitaxial strain stabilizes various ordered phases which give rise to a rich phase diagram below ~ 230 K. Among these phases, the chalcopyrite is dominant for $x = 0.5$, and two new, more complex, stable phases have been identified at different concentrations.

To appear in Phys. Rev. Lett., June 1994.

The RevTex manuscript can be obtained from n.marzari@phy.cam.ac.uk

Giant Magnetoresistance without Impurity Scattering

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Abstract

The transport properties of magnetic metallic multilayers are studied using first principles calculations whereby the *s*-electrons and the *d*-electrons, usually held responsible for conduction and magnetism respectively, are treated on an equal footing. A giant magnetoresistance of up to 120% is calculated for ballistic point contacts of Co/Cu multilayers. The effect can be explained as a slowing-down of the *s*-electrons by hybridization with *d*-electrons which are strongly reflected and partially localized by the spin-dependent interface potentials. The method should be a useful instrument in a systematic search for new materials for magnetoresistive applications.

(Submitted to Phys. Rev. Lett.)

Preprints can be obtained from schep@prl.philips.nl

Applications of Engel and Vosko's generalized gradient approximation in solids

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Abstract

Recently Engel and Vosko have proposed an alternative form of a generalized gradient approximation (GGA) [Phys. Rev. B47, 13164 (1993)] within density functional theory. This version of the GGA (EV93) was obtained by optimizing the exchange-correlation potential V_{xc} instead of the corresponding energy E_{xc} . We have applied this functional to various solids and found that equilibrium lattice constants generally are far too large in comparison to experiment so that the total energy aspect is unsatisfactory. However, EV93 describes FeO and CoO as antiferromagnetic insulators, while the local spin density approximation or the Perdew-Wang version of GGA yield a metallic ground state. EV93 favors magnetism, e.g. the spin susceptibility of V is increased, but Pd remains non-magnetic in agreement with experiment.

Phys. Rev. B (in press)

RevTex manuscript can be obtained from: heinz@olymp.theochem.tuwien.ac.at

Fermi Surfaces and Electronic Topological Transitions in Metallic Solid Solutions

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Abstract

Notwithstanding the substitutional disorder, the Fermi Surface of metallic alloys can be measured and computed. We show that, from the theoretical point of view, it is defined as the locus of the peaks of the Bloch Spectral Function (BSF). Such Fermi surfaces, on varying the atomic concentrations, may undergo changes of their topology, known as Electronic Topological Transitions (ETT). Thus, for instance, pockets of electrons or holes may appear or disappear, necks may open or close. ETTs cause anomalous behaviours of thermodynamic, transport and elastic properties of metals and constitute a fascinating field in the study of Fermi liquid systems. Although ETTs could be studied on pure systems as a function of the thermodynamic variables, nevertheless such a study would often require extreme conditions, and would lead to experimental difficulties. On the other hand, it is possible to explore the variations of atomic concentration, i.e. the valence electron per atom ratio, in metallic solid solutions with a relative experimental ease. In this paper we review the theoretical techniques for the determination of Fermi surfaces in metallic solid solutions and discuss some examples of ETTs, namely Li-Mg, Zr-Nb, Nb-Mo, Mo-Re, Ag-Pd, Cd-Mg, Ni-W and Ni-Ti alloys, also in connection with experimental data as thermoelectric power, resistivity, elastic constants and electron-phonon coupling and with the determinations of the electron momentum distribution function from Compton scattering and positron annihilation experiments. We show that the ab initio calculations of the electronic structure for the quoted systems, together with a careful determination of the BSF, are able to predict quantitatively ETTs at those concentrations where physical quantities display anomalies, so confirming directly ETT theory.

Submitted to Physics Reports (1994)

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