HCM Newsletter

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

Number 1   February 1994

Editorial

This is the first Newsletter of the HCM Network on *Ab initio (from electronic structure) calculation of complex processes in materials*. This Newsletter is distributed by e-mail only to the psik-network mailing list.

In general we would like all our newsletters to contain the following features: **News from the Network, News from the Working Groups, Preprint Information, Highlight of the Month, and Announcements**. Please let us have your input to this together with suggestions for additional features.

For the **Preprint Information** section we would like you to submit to us by e-mail a latex/revtex version of the *title page* of your manuscripts recently submitted for a publication. An abstract can be either short or extended version of the manuscript abstract, but cannot exceed one page. Moreover, the *title page* should contain the name of the journal to which you have submitted your manuscript and an e-mail address of the author from whom latex/revtex version of your manuscript could be obtained.

The purpose of the **Highlight of the Month** section is to comment on the most interesting of your recent manuscripts/publications in a fairly general way. The selection of the paper(s) for this section will be based upon the advice of the spokepersons of the working groups. We are expecting your suggestions for this section.

The first newsletter is very biased to our own interests. We make no excuse for this and we leave it up to you to submit your contributions to the Newsletter to make it more balanced with respect to the Network interests.

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

News from the Network

Since this is the first issue of the HCM Newsletter, it seems appropriate to re-introduce the Network. The Network consists of 12 working groups (enumerated below) run by a Network Management Board (NMB).

The NMB consists of:

		e-mail	fax
V. Heine	Chairman + H.d.	tcmsec@phx.cam.ac.uk	+44 223 337356
O.K. Andersen	Vice-Chairman + H.b.	andersen@radix2.mpi-stuttgart.mpg.de	+49 711 689 1632
W.M. Temmerman	Coordinator + H.e.	w.m.temmerman@daresbury.ac.uk	+49 711 689 1632
Z. Szotek	Secretary	dzidka@radix3.mpi-stuttgart.mpg.de	+49 711 689 1632
J. Martins	H.a.	jlm@pseudo.inesc.pt	+351 1 52 5843
A. Svane	H.c.	svane@dfi.aau.dk	+45 8612 0740
J.E. Inglesfield	H.f.	johni@sci.kun.nl	+31 80 652 120
B.L. Gyorffy	V.a.	blg@siva.bristol.ac.uk	+44 272 255 624
P. Dederichs	V.b.	iff140%djukfa11@earn-relay.ac.uk	+49 2461 61 2620
O. Bisi	V.c.	bisi@science.unitn.it	+39 461 88 16 96
M. Gillan	V.d.	pha71@seq1.keele.ac.uk	+44 782 711093
C. Koenig	V.e.	koenig@univ-rennes1.fr	+33 99 28 67 17
M. Finnis	L	finnis@finnis.mpi-stuttgart.mpg.de	+49 711 22 65 722
M. Scheffler		scheffler@fhi-berlin.mpg.de	+49 308305531
V. Van Doren		vancamp%banruc60@earn-relay.ac.uk	+32 321 80 217
J. Norskov		norskov@ltf.dth.dk	+45 459 323 99
C. Patterson		cpttrson@vax1.tcd.ie	+353 1 6711 759
F. Flores		fernando@uamc10.fmc.uam.es	+34 1 397 4950
N. Stefanou		nstefan@atlas.uoa.ariadne-t.gr	+30 172 34100
P.J. Durham	Consultant	p.j.durham@daresbury.ac.uk	+44 925 603634

The 12 working groups are:

		spokesperson
H.a.	Density-Functional Molecular-Dynamics Techniques	J Martins
H.b.	Muffin tin techniques	O.K. Andersen
H.c.	Improved Density Functionals	A. Svane
H.d.	Pseudopotential Techniques	V. Heine
H.e.	Algorithms for Parallel Computers	W. Temmerman
H.f.	Green's Function Techniques	J.E. Inglesfield
V.a.	Electronic Structure in the Normal and in the Superconducting State	B.L. Gyorffy
V.b.	Magnetism	P. Dederichs
V.c.	Reduced (0-1-2) Dimensionality	O. Bisi
V.d.	Oxide Materials	M. Gillan
V.e.	Molecules and Organic Solids	C. Koenig
L	Large Systems	M. Finnis

The NMB meets regularly to coordinate the activities of the working groups and decides on the Network budget. At its first meeting in Stuttgart on September 24, 1993 it set the budget for the period 1 January 1994 - 31 December 1996 as follows:

245 kECU   **working groups**
 75 kECU   **conference**
 60 kECU   **Network support**
 20 kECU   **NMB meetings**

The next NMB meeting will take place on March 3, 1994 in Paris and the minutes of these meetings will be circulated by e-mail to the whole Network.

E-mail is the network communication's highway and following network e-mail addresses might be of use:

	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

Finally, if the activities for which you joined the Network are not taking place, do not hesitate to e-mail the spokesperson of the appropriate working group or the coordinator.

News from the Working Groups

News from Working Group Ha:Density-Functional Molecular-Dynamics Techniques

The Ha group is organizing a computer course in Berlin in the week of October 3 to 7 for PhD students and post-docs that are interested in learning the techniques of ab-initio molecular dynamics based on the pseudopotential plane-wave method. Participants will learn how to use the fhi93cp program from Matthias Scheffler group. The course is organized by J.L. Martins, E. Pehlke, M. Scheffler, J. Hafner and G. Kresse. Applications should be sent no later than April 1st to Jose.L.Martins@inesc.pt
Jose L Martins

News from Working Group Hc: Improved Density Functionals

This working group is planning to hold a workshop in the near future.

News from Working Group He: Algorithms for Parallel Computers

Interest in a workshop was expressed by groups from Greece, the UK and Germany. A suitable location and time is being investigated. The subject of the workshop would cover parallel, distributed and vector computing and aims to display the varied experiences in electronic structure calculations in Europe.
Walter Temmerman

News from Working Group Hf: Green's Function Techniques

There has been some response in favour of a one-day or half-day meeting of the working group in MUENSTER, on FRIDAY 25th MARCH, at the end of the German Physical Society meeting. A suggested format would be presentations by each group for 15 minutes followed by discussion on collaboration. Whether we have a whole day or (more probably) a half-day depends on numbers.
John Inglesfield

News from Working Group Va: Electronic Structure in the Normal and in the Superconducting State

The Network nodes Bristol (Gyorffy), Stuttgart(Andersen), Daresbury(Temmerman) and Karlsruhe (Winter) are collaborating to implement the DFT-Bogoliubov-de Gennes equations for the YBCO systems.

News from Working Group Vb: Magnetism

This working group is organizing a workshop in Vienna from 28-31 May. More information can be obtained from Peter Weinberger (pw@eecws4.tuwien.ac.at)

News from Working Group L: Large Systems

My suggestion for a small workshop on Dynamics with O(N) Tight-Binding, henceforth to be called the DONTB workshop has been supported by groups in the UK, Finland and Greece and I have started to organise it. It will take place in Stuttgart on 11-12 April. There will be a small number of twenty minute talks and a lot of discussion. Topics to include:

1. Implementations of the tight-binding bond model

2. Implementations of other O(N) models

3. Comparison of k-space and real space methods

4. What are the prospects for parallel coding?

5. Can we benefit from sharing codes, developing new ones?

I expect about 7 overseas participants, and will ask them to apply for network funding individually and pay their own bills.
Mike Finnis

Electronic Structure of Cerium in the Self-Interaction Corrected Local Spin Density Approximation.

A. Svane.

Institute of Physics and Astronomy, University of Aarhus,

DK-8000 Aarhus C, Denmark

Abstract

The electronic structure of cerium is calculated in the self-interaction corrected local spin density approximation. In this formalism the electronic eigenstates may be described as either localized or delocalized. Two competing local minima of the total energy functional are found. The γ-phase is found to be excellently described with one f-electron per atom being localized. In contrast, the α-phase is best described with delocalized f-electrons. The total energy is approximately equal in the two phases allowing for a low-pressure transition between them in accordance with experiment.

On The Self-Interaction Corrected Local Spin Density Approximation.

A. Svane.

Institute of Physics and Astronomy, University of Aarhus,

DK-8000 Aarhus C, Denmark

Abstract

It is demonstrated that there exists no ambiguity in the definition of the self-interaction corrected local spin density approximation in density functional theory. This opposes the recent conclusion of Biagini (Phys. Rev. **B49**, 2156 (1994)), which we show is based on an ill-defined functional.

The SIC-LSD description of the $\gamma \rightarrow \alpha$ transition in Ce

Z. Szotek †, W.M. Temmerman ‡§†, and H. Winter §

† Max-Planck Institut für Festkörperforschung, Stuttgart, FRG

‡ SERC Daresbury Laboratory, Warrington, U.K.

§ Kernforschungszentrum Karlsruhe, INFP, Karlsruhe, FRG

Abstract

We show that, in contrast to the local spin density (LSD), the self-interaction corrected (SIC)-LSD provides correct description of the γ-phase of Ce metal. It correctly accounts for the volume and magnetic moment collapse at the $\gamma \rightarrow \alpha$ transition, in good agreement with experiment. The theoretical volume of the γ-phase is ~ 0.2 % smaller than the experimental volume, while the LSD underestimates by about 9–10 % the volume corresponding to the α-phase. The energy difference between the minima of the respective total energy curves is 5 mRy. A common tangent construction gives a *positive* transition pressure of ~ 17 kbar, as opposed to -8 kbar, the value obtained by extrapolating from the phase diagram to T=0 K. The theoretical volume collapse is ~ 23 %, as compared to the experimental values of about 15–17 %. Our results show that the strong hybridization effects of the f electrons are the driving force behind the $\gamma \rightarrow \alpha$ transition in Ce. This leads to an energy lowering of the non-magnetic state below the magnetic state at small volumes. These *ab initio* calculations do not discriminate between either the Kondo volume collapse model or the Mott transition model. They correctly account for the hybridization change at the transition, in agreement with both models, and lead to a small energy difference between the two phases. The large underestimation of the equilibrium volume of α-Ce could be interpreted as an indication of missing correlations due to the Kondo screening. Equally well, however, one could argue that LSD would normally overestimate the f-f hopping integral and bonding of such strongly correlated system as α-Ce. Therefore, at this stage one cannot draw final conclusions with respect to the nature and degree of localization of the $4f$ electrons in the non-magnetic α-phase.

The Structure of Special Grain Boundaries in α-Al$_2$O$_3$

Thomas Höche, Philip R. Kenway [1], Hans-Joachim Kleebe [2],

Michael W. Finnis and Manfred Rühle

Max-Planck-Institut für Metallforschung,

Institut für Werkstoffwissenschaft,

Seestraße 92, D-70174 Stuttgart, Germany

Abstract

With High Resolution Transmission Electron Microscopy we have studied the structure of the (bar1104) twin boundary in pure α-Al$_2$O$_3$. Two twin boundaries of this orientation were prepared in the form of diffusion- bonded bicrystals. In the second of these specimens, one of the surfaces to be bonded was predoped with Al. Two distinct boundary structures (labelled B and C) were identified in this specimen, one of which (C) was also observed in the first specimen. The commonest structure (C) exhibited continuous lines of intensity maxima through the boundary, whereas in the other structure (labelled B) these were broken by a parallel translation of the grains. The boundary was then simulated by atomistic relaxation, which also resulted in two mechanically stable structures similar to B and C. Finally an atomistic stucture was estimated by fitting simulated images to the experimental micrograph. The theoretical calculations were consistent with some features of the micrographs, notably the two translation states observed, but significant discrepancies remain. We discuss the likely sources of error.

(Submitted to J.Phys.Chem.Solids. The original was written with Microsoft Word 5.0 on a Macintosh but the figures are not digitized, so only old-fashioned preprints are available from finnis@finnis.mpi-stuttgart.mpg.de)

---

[1]now at: Merck, Sharp and Dohme Research Laboratories, Neuroscience Research Centre, Terlings Park, Harlow, Essex CM20 2QR, U K

[2]now at: Universität Bayreuth, Institut für Materialforschung, Ludwig-Thoma-Str. 36b, D-95440 Bayreuth, Germany

Plane dimpling and saddle-point bifurcation in band-structures of optimally doped high-temperature superconductors; a tight-binding model.

O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin.

Max Planck Institut für Festkörperforschung, D-70569 Stuttgart, FRG.

Abstract

We argue that extended saddle points observed at the Fermi level for optimally doped superconductors are essentially the bifurcated saddle points predicted by density-functional (LDA) calculations. Such saddle points are caused by the dimple of the CuO_2 planes and are enhanced by plane-plane hopping. Dimpling may provide a mechanism for pinning the Fermi level to the saddle points. Simple tight-binding Hamiltonians and analytical expressions for the constant-energy contours are derived from the LDA bands of $YBa_2Cu_3O_7$. In addition to the usual O2 x, O3 y, and Cu x^2-y^2 orbitals, we find that O2 z and O3 z are crucial and Cu s, xz, and yz important. The O z orbitals allow the $pd\sigma$ antibond to tilt with the dimple.

An Improved Tetrahedron Method for Brillouin-Zone Integrations

Peter E. Blöchl[a,b], O. Jepsen[b] and O.K. Andersen[b]

[a]IBM Research Division, Zurich Research Laboratory,

CH-8803 Rüschlikon, Switzerland

[b]Max-Planck-Institut FKF, Heisenbergstr. 1,

D-70569 Stuttgart, Germany

Abstract

Several improvements of the tetrahedron method for Brillouin-zone integrations are presented. 1) A translational grid of k-points and tetrahedra is suggested that renders the results for insulators identical to those obtained with special-point methods with the same number of k-points. 2) A simple correction formula goes beyond the linear approximation of matrix elements within the tetrahedra and improves the results also for metals significantly. For a required accuracy this reduces the number of k-points by orders of magnitude. 3) Irreducible k-points and tetrahedra are selected by a fully automated procedure, requiring as input only the space-group operations. 4) The integration is formulated as a weighted sum over irreducible k-points with integration weights calculated using the tetrahedron method once for a given band structure. This allows an efficient use of the tetrahedron method also in plane-wave-based electronic structure methods.

The Fermi surface of Pd$_2$Si

V.N. Antonov, B.Ya. Yavorsky, V.V. Nemoshkalenko

Institute of Metal Physics, Kiev 142, Ukraine

Vl.N. Antonov, O. Jepsen, O.K. Andersen

Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart,

Fed. Rep. Germany

E.G. Haanappel, M. Vosgerau, W. Joss, P. Wyder

Max-Planck Institut für Festkörperforschung,

High Magnetic Field Laboratory and

Centre National de la Recherche Scientifique

Boîte Postale 166, F-38042 Grenoble CEDEX 9, France

R. Madar and A. Rouault

Ecole Nationale Supérieure de Physique de Grenoble,

Laboratoire des Matériaux et du Génie Physique,

Boîte Postale 46, F-38402 Saint-Martin-d'Hères CEDEX, France

Abstract

A Fermi surface study of palladium disilicide is presented. Experimentally the Fermi surface and the cyclotron effective masses have been studied using the de Haas van Alphen (dHvA) effect. Theoretically the band structure of Pd$_2$Si has been calculated using the Linear Muffin-Tin Orbital method in Atomic-Spheres-Approximation (LMTO-ASA) . The Fermi surface consists of three small hole pockets, an open hole surface, and two large electron sheets. The calculated angular dependence of the extremal cross sections of the Fermi surface are in reasonable agreement with dHvA experiments. Some additional dHvA oscillations are predicted.

HIGHLIGHT OF THE MONTH

Comment on:

Electronic Structure of Cerium in the Self-Interaction Corrected Local Spin Density Approximation *by A. Svane*, to appear in Phys. Rev. Lett., February 21, 1994, and

The Self-Interaction Corrected Local Spin Density description of the $\gamma \rightarrow \alpha$ transition in Ce *by Z. Szotek, W.M. Temmerman, and H. Winter*, to appear in Phys. Rev. Lett., February 21, 1994

The $\gamma \rightarrow \alpha$ phase transition in Ce metal has been studied extensively both experimentally and theoretically. This transition is unique in being isostructural (fcc→fcc) and it is associated with ~15–17 % volume collapse, as well as, a magnetic moment collapse [1]. It has a phase boundary terminating at a critical point which makes Ce a special case among elemental metals. At low temperatures and normal pressures α-Ce is the stable phase. This transition has received a lot of attention throughout the years and several models have been proposed to explain it. The most well known are the promotional model [2], the Mott transition model [3], and the Kondo volume-collapse (KVC) model [4].

The promotional model involves a promotion of the Ce $4f$ electron to the $5d$ conduction-band state. However, this model is difficult to reconcile with the cohesive properties of Ce [3] as well as with photoemission data [5]. Moreover, positron annihilation experiments probing the electron density have not found any substantial difference in the number of $4f$ electrons across the transition [6]. This was confirmed by Glötzel [7] whose first local spin density (LSD) calculation showed no substantial change in the $4f$ occupation number. Similar conclusions could be drawn from the subsequent calculations performed within the

local density approximation [8]. However, none of those calculations could reproduce the characteristics of this first order isostructural transition, and no stable γ-phase was found. What those calculations showed, in agreement with experimental evidence, is the formation of a magnetic moment for the volumes in the neighborhood of γ-Ce, indirectly implying localized nature of the f electrons in this phase.

In the Mott transition model the $4f$ electrons are treated as localized and nonbonding in the γ-phase, whereas in the α-phase they are considered to be itinerant and bonding. This implies that the energy needed to destroy the f local moment in the γ-phase is surmounted at the phase transition by the energy gained on an f band formation in the α-phase. This model is consistent with positron annihilation experiments suggesting delocalization of the $4f$ electrons in α-Ce into a band state [6]. No quantitative description of cerium within the Mott transition picture at finite temperature has been presented.

In the Kondo volume collapse model [9] the transition is assumed to be governed by spin screening of the localized f-electrons by the (spd) conduction electrons. In this model the γ-phase consists of essentially unscreened localized moments, while the α-phase consists of screened moments. The screening of a localized f-electron is accomplished by the non-f valence electrons on the neighbouring atoms forming a spin singlet with the f-electron and is then controlled by the f-(spd) hopping matrix elements. This screening is well understood for an isolated localized moment [10] but till now the effect of a periodic array of local moments has not been described. In the calculation of the Kondo volume collapse model [9] it is assumed that the results for the single moment case (in particular the strong dependance of the screening energy on volume) can be carried over to the lattice case. With this assumption it has been shown that the detailed characteristics of the $\gamma \rightarrow \alpha$ phase transition, including the occurrence of a critical point, may be explained [9]. In accordance with the Kondo volume collapse model, the photoemission experiments on cerium are well accounted for with the Anderson impurity model [11]. Both the Mott transition model and the Kondo volume collapse model agree that the γ-phase of cerium consists of localized f-electrons, while the dispute is over the nature of the α-phase.

Eriksson et al. [12], by implementing the orbital-polarization formalism, involving orbital and spin quenching, have reproduced certain features of the $\gamma \rightarrow \alpha$ transition. In this formalism the itinerant states are used to describe both phases, and one deals with fourteen partially occupied $4f$ orbitals that sum up to one.

The papers by Svane and Szotek et al. apply an *ab initio* approach to the $\gamma \rightarrow \alpha$ transition in Ce, provided by the LSD and self-interaction corrected (SIC)-LSD formalisms. They concentrate on the first principles self-consistent total energy calculations as a function of the lattice parameter.

The self-interaction corrected local-spin-density approximation [13] is an *ab initio* electronic structure scheme, which describes static Coulomb correlation effects much better than the LSD approximation. This has been demonstrated in studies of the Hubbard model [14], in applications to 3d monoxides [15] and La_2CuO_4 [16] and hydrogen solid [17]. In the papers

commented upon here Svane and Szotek et al. demonstrate that this scheme is also capable of describing γ-Ce properly and in fact provides a unified *ab initio* framework for studying both the α-phase and the γ-phase of cerium.

In the SIC-LSD one subtracts from the LSD total energy functional E^{LSD} the self-Coulomb, $U[n_i]$, and self-exchange-correlation energy, $E_{xc}^{LSD}[n_i]$, for each occupied orbital, where n is the total spin-density of the electrons, while n_i is the spin-density of the i'th occupied electron orbital. The rationale is that E^{LSD} erroneously includes the self-interaction of each electron, which is then corrected for in the SIC-LSD energy functional E^{SIC}. The self-interaction vanishes for extended states, for which reason the SIC-LSD energy functional is identical to the LSD energy functional in the entire region of configuration space corresponding to Bloch-like one-particle wavefunctions. The possibility exists, however, that different local minima of E^{SIC} containing localized wavefunctions can be found with a lower total energy than the LSD-like local minimum.

The two papers differ in the implementation of the SIC-LSD formalism. Svane has implemented the SIC-LSD approximation within the linear-muffin-tin-orbital (LMTO) method in the tight-binding representation [18] and with the atomic-spheres approximation (ASA). The SIC-LSD energy functional is minimized by using a simple steepest descent iterative scheme for the localized states and subsequently solving the secular equation for the itinerant states in the subspace orthogonal to the localized states. Szotek et al. have taken an advantage of the unified Hamiltonian concept [19] and converted the minimization of the SIC-LSD energy functional into a standard eigenvalue problem which by making use of crystalline symmetry they have solved applying the standard unscreened linear-muffin-tin-orbitals method, with the atomic sphere approximation [20]. With respect to technical details of the calculation both papers differ in the choice of the energy panels and the symmetry of the f band states to be self-interaction corrected. Despite that, and what is most reassuring, both papers reach very much the same conclusions concerning the important physical issues of Ce.

These papers demonstrate, for the first time, that it is possible from first principles calculations to obtain two energy minima corresponding to the α-phase and the γ-phase , respectively. Since, both curves represent local minima of the same energy functional a phase transition is predicted to take place. It is significant that the energy difference between the two minima, corresponding to either localized or delocalized f-electrons, is in mRy range allowing for a low-pressure transition between the phases, in agreement with experimental evidence. Disregarding some sensitivity of the relative positions of the LSD and SIC-LSD total energy minima and the actual value of the transition pressure to the choice of the energy panels and basis functions these *ab initio* calculations correctly reproduce the crucial characteristics of this first order $\gamma \rightarrow \alpha$ transition, and especially, the SIC-LSD describes the γ-phase extremely well. The stiffness of both the α-phase and the γ-phase around $P = 0$ as well as the $P = 0$ volume of the α-phase are not well reproduced within the present formalism which may be taken as an indication that still some effects, as e. g. Kondo screening, have not been properly described. These calculations correctly account for the disappearence of

the magnetic moment at the transition and give the theoretical volume collapse of $\sim$23-24 %. The reason for the overestimation of the volume collapse primarily lies in the failure of the LSD to better describe α-Ce. The LSD fails to describe the α-phase as well, as the SIC-LSD describes the γ-phase. This is probably not surprising due to the fact that the α-phase is still a strongly correlated system, and the LSD would substantially overestimate the value of the f-f hopping integral. However, the LSD has been successful in describing high-pressure phases of Ce [21], suggesting the sensitivity of this hopping integral to the volume. In the γ-Ce the $4f$ states are split into the occupied states, occuring at about –7.5 eV below E_f, and the unoccupied states at about 1 eV above E_f. These papers show that the strong hybridization effects of the f electrons are the driving force behind the $\gamma \rightarrow \alpha$ transition in Ce, in agreement with both the KVC and the Mott transition models. Suffices to say, that the SIC-LSD provides a correct description of the γ-phase and leads to a small energy difference between the two phases. The large, $\sim$10 %, underestimation of the equilibrium volume of α-Ce could be interpreted as an indication of missing correlations due to the Kondo screening. Equally well, however, one could argue that LSD would normally overestimate the f-f hopping integral and bonding of such strongly correlated system as α-Ce. The inclusion of Kondo screening of the localized moments within the SIC-LSD description is a difficult task. The SIC-LSD formalism relies, as the LSD, on a single Slater determinant description. One may presume quantum fluctuations to be improperly described in cases where they are significant. Therefore, at this stage one could not draw final conclusions with respect to the nature and degree of localization of the $4f$ electrons in the non-magnetic α-phase. Nevertheless, the main result of these papers, i.e., a succesful *ab initio* description of the γ-Ce , is an important contribution to a better understanding of the $\gamma \rightarrow \alpha$ phase transition in Ce.

References

[1] *Handbook on the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneidner, Jr., and L. Eyring (North Holland, Amsterdam, 1979), Vol. I.

[2] W. H. Zachariasen (unpublished) quoted in A. W. Lawson and T. Y. Tang, Phys. Rev. **76** 301 (1949); L. Pauling, J. Am. Chem. Soc. **69**, 542 (1947).

[3] B. Johansson, Philos. Mag. **30**, 469 (1974).

[4] J. W. Allen and R. M. Martin, Phys. Rev. Lett. **49**, 1106 (1982); R. M. Martin and J. W. Allen, J. Magn. Mag. Mater. **47 & 48**, 257 (1985); M. Lavagna, C. Lacroix, and M. Cyrot, Phys. Lett. **90A**, 210 (1982); J. Phys. F **13**, 1007 (1983).

[5] E. Willoud, H. R. Moser, W.-D. Schneider, and Y. Baer, Phys. Rev. B **28**, 7354 (1983).

[6] D. R. Gustafson, J. D. McNutt, and L. O. Roelling, Phys. Rev. **183**, 435 (1969); A. M. Boring, C. Y. Huang, K. A. Gschneidner, Jr., J. D. McGervey, M. Pavifrahi, and S. G. Usmar, J. Magn. Mag. Mater. **37**, 7 (1983).

[7] D. Glötzel, J. Phys. F **8**, L163 (1978).

[8] W. E. Pickett, A. J. Freeman, and D. D. Koelling, Physica **120B**, 341 (1980); B. I. Min, H. J. F. Jansen, T. Oguchi, and A. J. Freeman, Phys. Rev. B **34**, 369 (1986).

[9] J. W. Allen and R. M. Martin, Phys. Rev. Lett. **49**, 1106 (1982); J. W. Allen and L. Z. Liu, Phys. Rev. **B46**, 5047 (1992).

[10] See e.g. P. Fulde, J. Keller and G. Zwicknagl, Solid State Phys. **41**, 1 (1988).

[11] L. Z. Liu, J. W. Allen, O. Gunnarsson, N. E. Christensen and O. K. Andersen, Phys. Rev. **B45**, 8934 (1992).

[12] O.Eriksson, B. Johansson, and M. S. S. Brooks, Physica B **163**, 337 (1990).

[13] J. P. Perdew and A. Zunger, Phys. Rev. **B23**, 5048 (1981).

[14] A. Svane and O. Gunnarsson, Phys. Rev. **B37**, 9919 (1988); A. Svane and O. Gunnarsson, Europhys. Lett. **7**, 171 (1988).

[15] A. Svane and O. Gunnarsson, Phys. Rev. Lett. **65**, 1148 (1990); Z. Szotek, W. M. Temmerman and H. Winter, Phys. Rev. B **47**, 4029 (1993).

[16] A. Svane, Phys. Rev. Lett. **68**, 1900 (1992); W. M. Temmerman, Z. Szotek and H. Winter, Phys. Rev. B **47**, 11533 (1993).

[17] A. Svane and O. Gunnarsson, Solid State Commun. **76**, 851 (1990).

[18] O. K. Andersen, Phys. Rev. **12**, 3060 (1975); O. K. Andersen, O. Jepsen and D. Glötzel, in *Highlights of Condensed Matter Theory*, International School of Physics 'Enrico Fermi', Course 89, ed. by F. Bassani, F. Fumi and M. P. Tosi, (North-Holland, Amsterdam, 1989), p 59.

[19] R. A. Heaton, J. G. Harrison, and C. C. Lin, Phys. Rev. B **28**, 5992 (1983).

[20] O.K. Andersen, Phys. Rev. B **12**, 3060 (1975).

[21] J. M. Wills, O. Eriksson, and A. M. Boring, Phys. Rev. Lett. **67**, 2215 (1991); O.Eriksson, J. M. Wills, and A. M. Boring, Phys. Rev. B **46**, 12981 (1992).

ANNOUNCEMENT

European Research Conference
ELECTRONIC STRUCTURE OF SOLIDS
"Dynamics and Excitations"

Gausdal, Norway 27.8. - 1.9. 1994

Following the successful meetings in Cambridge (1992) and Porto Carras (1993), the 1994 ERC, sponsored by the European Science Foundation, will be held in a beautiful mountain resort in Norway. The program will follow the format of the previous meetings. There will be a number of invited talks with ample time for critical discussion. A poster session will be arranged. There will not be any formal proceedings.

The topics to be discussed include
  density-functional theory and its extensions
  excitations and charge transfer
  novel spectroscopies
  dissipation and tunnelling
  dynamical simulations
  applications to solids and surfaces

The preliminary list of invited speakers includes

O. Gunnarsson	N. Martensson
U. Landman	N.D. Lang
L. Fritzsche	P. Hedegard
P. Echenique	A. Liebsch
M. Persson	G. Wahnstrom

and (to be confirmed) B. Cooper, J.W. Wilkins, M. Steiner, F. de Sette, P. Weinberger, R. Godby, G. Sawatzky.

More details of the program and instructions on how to apply for participation will be sent out shortly by the European Science Foundation. Enquiries should be sent to the Conference Chairman, using the e-mail address erc94@hugo.hut.fi.

Looking forward to meet you in Gausdal,

Sincerely

Risto Nieminen	Balazs Gyorffy
Conference chairman	vice-chairman

Ab-initio molecular-dynamics calculations of structural, elastic, and vibrational properties of poly-atomic systems

In this course the basic concepts of density-functional theory calculations will be explained, and an introduction to the computer program fhi93cp will be given. This program allows calculations for molecules, perfect crystals, defects in crystals, and crystal surfaces. Although it is feasable to treat systems with more than 100 atoms, the hardware needs are just a 12 k ECU workstation.

The course will start on Monday morning, October 3, and will end on Friday evening, October 7, 1994. Every morning there will be lectures on density-functional theory, the local-density approximation for the exchange-correlation energy-functional, the generalized gradient approximation, the ab-initio pseudopotential approach, molecular dynamics, etc. The afternoon is devoted to active computations of simple physical properties, using the computer code fhi93cp. Examples of computations may include:

- bonding and vibrational properties of simple molecules (e.g. Si_2 and C_2)

- lattice constant, bulk modulus, and phonons of Si.

- structural phase transitions (Si, diamond $\leftrightarrow$ β-tin structure)

PhD students and postdocs who are interested in attending this course should send their applications to

Dr. José Luís Martins

INESC

Rua Alves Redol 9

Apartado 13039

P-1000 Lisbon, Portugal

fax: +351-1-52 58 43

e-mail: Jose.L.Martins@inesc.pt

The letter should include a description of a scientific project which the applicant plans to study subsequently to the course. The length of this description should be no longer than 1-2 pages. Furthermore it would be good to include two support letters from established scientists.

The course will take place at the Fritz-Haber-Institut of the Max-Planck-Gesellschaft in Berlin (Germany). Lodging will be arranged in a hotel (DM 75,–/night incl. breakfast). Participants belonging to the Human Capital and Mobility Network "Ab initio (from electronic structure) calculation of complex processes in materials" can receive upon request financial support for the local as well as for the travel expenses.

Applications should be sent no later than April 1st by e-mail or fax as well as by normal mail to Dr. J.L. Martins. Because the number of participants will be limited to 20 persons, we will most likely have to reject some applications. Information about acceptance or non-acceptance will be sent out by late April.

Applicants are expected to have a profound knowledge of quantum mechanics and the physics and chemistry of bonding. Furthermore a good knowledge of FORTRAN and UNIX is required. All this should be stated clearly in the application.

The course will be organized by Drs. J.L. Martins, E. Pehlke, M. Scheffler, J. Hafner and G. Kresse, together with significant support from the Theory Department of the Fritz-Haber-Institut.

Some ideas about the computer code and its applicability can be found in the following references:

1. R. Stumpf and M. Scheffler: "Simultaneous calculation of the equilibrium atomic structure and its electronic ground state using density-functional theory", Computer Physics Communications (in press).

2. J. Dąbrowski, E. Pehlke, and M. Scheffler: "Calculation of surface stress anisotropy for the buckled Si (001)(1×2) and p(2×2) surfaces", Phys. Rev. B, Feb. 15 (1994).

3. J.L.A. Alves, J. Hebenstreit, and M. Scheffler: "Calculated atomic structures and electronic properties of GaP, InP, GaAs and InAs (110) surfaces", Phys Rev. B **44**, 6188 (1991).

4. J. Neugebauer and M. Scheffler: "Adsorbate-substrate and adsorbate-adsorbate interaction of Na and K adlayers on Al (111)", Phys. Rev B **46**, 16067 (1992).

5. E. Pehlke and M. Scheffler: "Evidence for site-sensitive screening of core-holes at the Si and Ge (001) surface", Phys. Rev. Lett. **71**, 2338 (1993).

6. R. Stumpf and M. Scheffler: "Theory of self-diffusion at and growth of Al (111)", Phys. Rev. Lett. **72**, 254 (1994).

The computer code together with reference [1] can be obtained by the following procedure:

```
          ftp 141.14.129.9
Name:     anonymous
password: (none)
          cd pub/physics/fhi93cp
          bin
          get fhi93cp.tar.Z
          quit
```
then you continue on your machine:
```
          uncompress fhi93cp.tar.Z
          tar -xvf fhi93cp.tar
```
to start the program change to directory `Dfhi93cp/Drun` and enter
```
          run_fhi93cp
```

The LaTeX file of Ref. [1] is : `cpc3.tex`