HCM Newsletter

Ψ_k Network

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

Number 2 April 1994

Proposal: ERB4050PL930589
Contract: ERBCHRXCT930369

Coordinator: Walter Temmerman
E-mail: psik-coord@daresbury.ac.uk

Editorial

In this Newsletter we have different sections as compared to the previous Newsletter. Most importantly, we have a **Message from the Network's Chairman** concerning our **Preprint Section**. Although this section has proven very useful, we do not receive enough input from you. Those who sent their abstracts for the first Newsletter have received many requests for the preprints from all over the world.

In this Newsletter there is also the **Chairman's Message about how to get your hands on some of the Network's money**.

In place of the **News from the Working Groups** we include the minutes of the last Network's Management Board (NMB).

In the **Announcement Section** there is an information on the **Hands-on TB-LMTO Workshop** to take place at the Max-Planck-Institute FKF in Stuttgart in October. There you can also find a second announcement of the workshop on **ELECTRONS IN DIFFERENT DIMENSIONS** which will take place in May in Varenna (Italy). Moreover, we also include a preliminary announcement of the *Third Aarhus Workshop on* **Quantum Theory of Solids: Improved Density Functionals** to take place in June, and an announcement of the summer school on **Nanoscale Materials Physics** to take place in August.

Finally, we include the full **list of the subscribers** to our ψ_k-Network. It is structured around the countries and nodes. We have marked the nodes which are not funded but are interested in collaborations with the Network using their own funds. Please, contact us if you would like to be included into our list.

Our Network has been given the possibility of financing the participation of organisations and/or scientists of Central and Eastern Europe and the New Independent States of ex-USSR. If you want more information contact us. As usually, in these matters with Brussels we need to react fast.

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

Chairman's Message about Preprint Information

President Kennedy made a famous remark, which when suitably adapted would run *"Think not just about what the Network can do for you but also what you can do for the Network"*.

Please submit preprint information about ALL papers written/submitted after 1st January 1994. We want the Network to be renewed after the present 3-year run, and the sharing of preprint information is an important activity which we will be pointing to. So, please everyone do it.

The procedure is:

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.

Volker Heine

Chairman's Message about how to get your hand on some Network money!

The Network is up and running. So, now is the time to start that collaboration which you always wanted to but never had money for. Or maybe you need to consult someone to learn about something for your own research: go and visit the people, and put their names on the final resulting paper; that counts as collaboration. Last summer you had all the e-mail about what everyone is doing, and in this Newsletter you have the list of fax numbers and e-mail addresses. In the last Newsletter there was a list of the leaders of the Working Groups of the Network: they can also help you with information.

The procedure for requesting the money and then getting it is as follows.

1. Ask for the money by sending an e-mail to the Management Board saying: how much money you need, which node is collaborating with which node, three or four lines about the scientific purpose of the visit, and a suggestion which of the 12 Working Groups the project best fits under. We have agreed to be flexible about interpreting the areas covered by the Working Groups so, that more or less anything can be fitted in. If in doubt ask the secretary of the NMB or relevant Working Group coordinator.

2. Please see Minutes of the NMB in this Newsletter for special rules when you are discussing a collaboration within some other conference. Also, note the limit of 40 ECU per day for subsistance, and of course economy class travel.

3. If there has been no objection by a NMB member within two weeks, then the request is automatically approved.

4. After the visit you claim the money by filling in a special form available from the secretary of the NMB.
You **MUST** at the same time submit a scientific report of a few lines about your consultation. The reports are needed for Brussels.
Repeat in your report the total amount being claimed, the collaborating nodes, and the relevant Working Group.

Volker Heine

News from the Network

The Network's Management Board meeting took place on March 3, 1994 in Paris at the Laboratoire de Chimie Physique-Matiere et Rayonnement, Universite Pierre et Marie Curie. The matters of the Network and the activities of the Working Groups were discussed quite extensively. Therefore, in this Newsletter we include the minutes of these meeting to keep you well informed on what happens within the Network. Obviously, the minutes replace our section **News from the Working Groups**, and also give good account of what you would normally find in the present section.

The next NMB meeting will take place on November 4, 1994 also in Paris. At this meeting the NMB will discuss in detail the Network's conference, which is planned for June 1996.

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**

Minutes of the Network Management Board (NMB): the chronological report of the 2nd NMB Meeting on March 3, 1994 at the Laboratoire de Chimie Physique-Matiere et Rayonnement, Universite Pierre et Marie Curie in Paris

Present: O.K. Andersen, O. Bisi, P. Dederichs, M. Finnis, B.L. Gyorffy, V. Heine (chairman), J. E. Inglesfield, C. Koenig, J. L. Martins, N. Stefanou, A.Svane, Z. Szotek, W.M. Temmerman (coordinator)

Apologies: P.J. Durham, F. Flores, M. Gillan, J. Noerskov, C. Patterson, M. Scheffler, V. Van Doren

1 Introductory Matters

The meeting was chaired by Volker Heine. The minutes of the previous meeting, which had taken place on 24th September 1993 at the MPI FKF in Stuttgart, were accepted with no corrections.
Volker Heine thanked Walter Temmerman for the enormous amount of work that he had put into making the Network to work. The chairman asked that to be recognized in the present minutes.
Volker Heine announced that in order to release Walter from that load of work Z. (Dzidka) Szotek has joined the NMB as a scientific secretary, on a part time basis. Till the end of March, 1994 her position has been subsidised by MPI FKF in Stuttgart. From May onwards, Daresbury Laboratory will pay part of her salary, covering her research and including all overheads, the other part will come from the Network. The contributions to the Network, from MPI FKF in Stuttgart and Daresbury Laboratory, should be acknowledged.
Walter Temmerman, thanked Coryn Hague for great help in organizing and hosting the present meeting at the Laboratoire de Chimie Physique-Matiere et Rayonnement in Paris.
Dzidka Szotek spoke about the HCM Newsletter, asking all the spokespersons for contributions to secure its regular publication. It has been suggested, that it might be too ambitious to publish the HCM Newsletter every month, and it was settled to publish it every 2 months. The first HCM Newsletter, of February 1994, was well received by the NMB. Volker Heine suggested to change the order of Newsletters' content in future editions. Namely, the announcements should come straight after the news from the Working Groups, followed by the highlight of the month section, and at the end one should include the preprint information. It was suggested that the whole Network should be encouraged to send, to the future newsletters, the first pages of the manuscripts sent for publication. It was concluded that a special chairman's message on the subject to the whole Network was needed.

Action: **Volker Heine would send a special message to the whole Network concerning the first manuscript pages for the preprint section of the Newsletter.**

2 Working Groups

The present spokespersons of the Working Groups presented brief reports on their groups activities.

(H.a.) Density-Functional Molecular-Dynamics Techniques (J. L. Martins)

Jose L. Martins spoke about the computer course to be organised in Berlin on the usage of the molecular dynamics-pseudopotential code developed by the group of Matthias Scheffler. The course is to be restricted to 20 participants with priority given to Europeans. The cost is estimated to be about 12000 ECUs, i.e. ~600 ECUs per Network participant. A special hotel deal of 75 DM can be arranged.

With respect to the above it was questioned whether 40 ECUs should be sufficient to cover participants' accomodation in Berlin, where no cheap student accommodation is available. The final decision was that one should stick to the sum of 40 ECUs, however, allowing to increase it in special cases.

(H.b.) Muffin tin techniques (O.K. Andersen)

Ole K. Andersen announced a hands-on course on the TB-LMTO code to be organised in the near future (preasumably in October) for about 10-20 participants in Stuttgart. The code is the latest, standard code of the Stuttgart group. It was suggested to make the program available by ftp and to make the deadline for participation in the workshop not sooner then June 1, 1994.

(H.c.) Inproved Density Functionals (A. Svane)

Axel Svane reported on the two-day workshop which is planned to take place in Aarhus in Denmark. It should bring together people from the LDA+U, SIC-LDA (LSD), GGA, GW, and H-F clubs. He asked the board for an input concerning other areas of interest in this respect. There have been no applications for money to support short collaborative visits within the group as yet.

It was suggested to invite to the workshop M. Foulkes, Dovesi, and somebody to talk about Gutzwiller-correlated wave functions.

(H.d.) Pseudopotential Techniques (V. Heine)

Volker Heine reported that nothing much has happened within the group since the Network had been funded. It has taken 4 manyears in Cambridge to develop and optimise generation of pseudopotentials. A small hands-on summer school for that is being considered. Another technical development in Cambridge is the calculation of energies and forces in metallic systems with a smaller number of k-points than previously.

(H.e.) Algorithms for Parallel Computers (W. Temmerman)

Walter Temmerman reported, that several nodes within this Working Group expressed an interest in organising a workshop devoted to vector, massively parallel and distributed computing (for example the Stuttgart group has a very good experience with it). B. Ginatempo from Messina has agreed to organise such a workshop in the near future. It is to focus both on the hardware and software.

It was suggested that parallel computing develops and changes so fast that it would be of interest to invite some computer specialists to such a workshop. It was also mentioned that massively parallel computers are working very well for lattice statistical applications. In case of pseudopotential applications they can distribute the whole wavefunction over the processors of the massively parallel machine. Although in many applications massively parallel machines have not been too successful, they would be of interest for a topic of such a workshop. It was suggested that it would be useful to publish in our newsletters people's experiences concerning running codes of interest on a variety of parallel/distributed machines.

(H.f.) Green's Function Techniques (J.E. Inglesfield)

John E. Inglesfield has reported that a collaboration between Nijmegen (J.E. Inglesfield) and Dublin (C. Patterson) has been started. Moreover, this Working Group is going to hold a half-day meeting attached to the March Conference of the German Physical Society in Münster. It is expected that this meeting will not use much of the Network's financial resources. It was suggested that H. Skriver should be invited to the meeting organised in Münster. John E. Inglesfield asked whether the KKR-CPA community is happy to belong to this Working Group. On behalf of the KKR-CPA community Balazs L. Gyorffy said yes.

(V.a.) Electronic Structure in the Normal and in the Superconducting State (B.L. Gyorffy)

Balazs L. Gyorffy has reported on the main activities of this Working Group which concentrate mostly on the calculations for the superconducting state and include: solving Hartree-Fock-Gorkov equations, solving Tight-Binding type equations, solving the Bogolubov-de Gennes equations coupled with Maxwell's equations. Following the tradition, a Bogolubov-de Gennes Day in Bristol or Stuttgart is planned. There has also been some interest expressed by Würzburg group, so this meeting is hoped to extend the existing Bristol -Daresbury-Sheffield-Stuttgart collaborations to other groups. It is also planned to invite scientists from outside the Network.

Action: Volker Heine encouraged Balazs L. Gyorffy to write an article for the Highlight of the Month section of the Newsletter on the main topic of this Working Group.

(V.b.) Magnetism (P. Dederichs)

Peter Dederichs reported that some genuine collaborations are starting with Bristol (a short visit of E. Bruno to be funded by the Network) and other groups. Moreover, a workshop is to take place in May in Vienna. It is mostly subsidised by the Austrian Group, however, about 3000 ECUs from the Network would be needed to pay for some of the invited people (eg. B. Johansson from Sweden). Money would be needed to fund the attendance at a satellite Network meeting of the Düsseldorf conference in August 1994. Money from the Network would also be needed for organising a workshop attached to the 1995 ERC conference in York.

(V.c.) Reduced (0-1-2) Dimensionality (O. Bisi)

As reported by Olmes Bisi no requests for the money has been received yet. This Working Group is concerned with very different areas of research and collaborations are hard to develop. Much more work is needed to attract people to form genuine collaborations. A workshop is planned in Varenna, so anybody interested in collaborations could join.

(V.d.) Oxide Materials (M. Gillan)

Due to the abscence of Mike Gillan, no report has been given.

(V.e.) Molecules and Organic Solids (C. Koenig)

Christine Koenig summarised the main points on which the research of this Working Group is concentrated. Of interest are molecular crystals which are a new subject. It requires a lot of computing power. It deals with non-spherical potentials, a correct treatment of the interstitial region is essential, as is the choice of the exchange-correlation potential. Due to the latter there is an interest in collaborations with the H.c Working Group, and a wide participation in the H.c group workshop is planned. Possible collaborations could involve Zürich, Basel, Philips, Vienna, Rennes and Konstanz. This Working group is not planning to organise any workshops. Short visits between C. Koenig, K.-H. Schwarz and P. Blöchl are planned and are to be funded by the Network. It was suggested to involve chemists in collaborations, since they are interested in using LDA + GGA.

(L) Large Systems (M. Finnis)

Mike Finnis reported on the workshop on Tight-Binding code to be held in Stuttgart this April. It has generated a lot of interest, however, mostly from outside the Network. About 3300 ECUs would be needed to fund invited speakers. Briefly, the way of funding outside people as consultants was discussed.

3 Network Conference

Ole K. Andersen (the conference chairman) proposed Schwäbisch Gmund (about 15 km from Stuttgart airport) for a place of the conference. The available accomodation is expected to cost about 60-120 DM/night.
He outlined how the conference could be organised with respect to plenary, invited, contributed talks and posters. Eight plenary lectures and $\sim$16 symposia, arranged by the Working Groups of the Network, are planned. The conference would be run in at most three, preferably two, parallel sessions. Every participant should be allowed to contribute a talk or a poster.

The NMB discussed whether there should be contributed talks or posters only, with reserved slot of time. The agreement was that there should be contributed talks as well as the posters and that the late evening session would be reserved for posters. It has been agreed, that the conference should have its specific character, and should not be organised around particular Working Groups. It should be accessible to a general public. There should be no proceedings of the conference. It has been suggested that such a big conference should be organised every three years.

The first Network's conference, will be organized, presumably in June 1996 and its duration is to be four days with expected attendance of ∼300 participants. It has been suggested to postpone the ERC conference of 1996 till the year after.
Details concerning the final structure and name of the conference are to be discussed at the next NMB meeting. The general feeling was that the name of the conference should be related to the ψ_k-Network. Also, it has been agreed that at the next NMB meeting a proper announcing poster would be designed and decisions would be taken on the plenary/invited sessions, their speakers etc.

Agenda for the next NMB meeting:

1. To discuss the conference name
2. To discuss the conference procedure, invited speakers, etc.
3. To design a poster announcement of the conference
4. To discuss the budget and see if other sources are available

Action: Volker Heine offered to discuss the postponement of the ERC conference of 1996 with the relevant people.

Action: The whole NMB should look into the budget matters and seek other possible sources of funding for the conference.

4 Wider Participation

It has been established that the groups from Austria and Finland received state funds for collaborations with the Network. Switzerland is hoped to receive money shortly. It has been decided that groups from Trieste, Lausanne, Uppsala, Göteborg and Lund should be encouraged to tighter collaborations with the Network and put on the e-mail list.

Action: J. L. Martins, O. Bisi and A. Svane have volunteered to make contacts with those groups, getting their e-mails, etc.

5 Budget

It has been agreed that wider and more detailed estimates of expected spendings from Working Groups would be needed. The issue of a Working Group organised workshop/satellite

meeting attached to a conference was settled as follows:

1 If the meeting lasts at least one full day one can reclaim full costs.

2 If the meeting lasts half a day, only half of the costs can be claimed; in this case, however, there should be a substantial amount of scientific discussions with other participants.

6 Next NMB meeting

It has been agreed that the next meeting is to take place on Friday, November 4, 1994, again at the Laboratoire de Chimie Physique-Matiere et Rayonnement, Universite Pierre et Marie Curie in Paris. A general consensus was that due to possible e-mail saturations at least one-two meetings of the NMB a year are needed to discuss important issues of the Network.

Action: Ole K. Andersen suggested that everybody should do much more homework for the next meeting.

Action: Z. Szotek/W. Temmerman to take care of the organisation of the next meeting.

Stuttgart, 15 March 1994

Dzidka Szotek

Announcement of the course:

Hands-on the TB-LMTO computer program.

Max-Planck-Institut FKF, Stuttgart, October 24-28, 1994

In this course the principles of the linear muffin tin orbital (LMTO) method will be explained, the latest version of the LMTO-ASA computer code will be described, and the use of the program will be practiced.

This version of the LMTO program

- uses the tight-binding (TB) representation of the LMTO method
- has down-folding capability which enables *ab initio* construction of minimal basis sets, simple TB-hamiltonians and automatic avoidance of ghost bands
- can use non-zero (positive or negative) kappa^2, (i.e. is KKR-equivalent).
- contains an automatic procedure for packing space with spheres
- uses the most accurate tetrahedron method for k-space integration.
- has several new features for analyzing the results, e.g. for plotting the full charge density, plotting fat (orbital projected) bands, and plotting ELF (electron localization functions).

Applications should be send to:

Ove Jepsen, Max-Planck-Institut FKF, Heisenbergstr. 1, D-70569 Stuttgart, Federal Republic of Germany. FAX: +711-689-1632 e-mail: jepsen@radix1.mpi-stuttgart.mpg.de

no later than July 1st 1994.

The application should contain a short resume of background and previous experience.

The course will take place at the Max-Planck-Institut für Festkörperforschung in Stuttgart. Participants belonging to the Human Capital and Mobility Network "Ab initio (from Electronic Structure) Calculation of Complex Processes in Material" can obtain financial support.

The number of participants is limited to 10.

Applicants are expected to have some knowledge of UNIX and in particular of a UNIX editor. No programming experience is necessary for the course.

The course will be organized by O. Jepsen, A. Burkhardt, G. Krier, and O.K. Andersen.

Second Announcement

Workshop on

ELECTRONS IN DIFFERENT DIMENSIONS
May 8-14, Varenna, Villa Monastero, Italy

Program

The workshop will focus 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 morning sessions will be devoted to more general lectures whereas the afternoon sessions will be reserved for more specialized seminars.

The list of speakers includes

- J. Fink (Dresden), A. Liebsch (Juelich), G. Senatore (Trieste) and F. Toigo (Padova) for the electron gas;
- T.P. Martin (Stuttgart) for the quantum wells;
- O. Bisi (Trento), H. Lueth (Juelich) for the quantum wires;
- K. Ensslin* (Munich), P.E. Lindelof (Copenhagen) and S. Stringari (Trento) for the quantum dots;
- R. Ferrari (Trento) and I. Kukuskin (Moscow) for the quantum Hall effect;
- G. Bachelet (Rome), C. Bréchignac (Orsay), M. Broyer (Lyon), W. Ekardt (Berlin), C. Guet (Grenoble), H. Haberland (Freiburg), M. Manninen (Copenhagen), J. Pacheco (Coimbra) and Ll. Serra (Mallorca) for clusters.

Location

The seminar will be held at Villa Monastero in Varenna. Varenna is a small village on the lake of Como and is directly connected with Milano by train (line Milano-Sondrio, about one-hour trip). Information on the train schedule are given below. Participants are expected to arrive in Varenna on Sunday afternoon.

Registration

More than 30 persons have already confirmed their participation to the workshop. Any other person interested in attending the workshop is kindly requested to contact the organizers as soon as possible.

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. Please contact O. Bisi (Bisi@science.unitn.it).

E. Lipparini, Dipartimento di Fisica, Universita' di Trento, Povo, Trento, Italy.
A. Vitturi, Dipertimento di Fisica, Universita' di Padova, Via Marzolo 8, Padova, Italy.
E-mail Lipparini@science.unitn.it
FAX 0461 - 881696

Train Schedule (from central station of Milano)

Milano	Varenna
9.00	10.17
12.05	13.09
14.05	15.14
16.05	17.06
18.03	19.12
19.08	20.12
20.05	21.03
21.20	22.47

* Not yet confirmed

Preliminary announcement, March 21, 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

Invited Speakers include:

J. Zaanen, Leiden,	on	*LDA+U*
W. Temmerman, Daresbury,	on	*Self-Interaction Corrections*
L. Severin, Darmstadt,	on	*Orbital Polarisation Schemes*
K.-H. Schwarz, Wien,	on	*Gradient Corrections*
E. K. U. Gross, Würzburg,	on	*Time-dependant DFT*
M. Foulkes, London,	on	*Quantum Monte Carlo*
O. Eriksson, Uppsala,	on	*Gradient Corrections*
M. Causá, Torino,	on	*Hartree Fock*
F. Aryasetiawan, Lund,	on	*GW*
V. Anisimov, Ekatarinenburg,	on	*LDA+U*

The time table leaves open a few slots for contributions from members of the Ψ_k HCM Network, Working Group H.c. (Improved Density Functionals), as well as others. If you would like to contribute, send me (no later than April 15th) an email, and I will fit you into the final programme. The time allotted to each contributed talk will depend on the number of contributions. Registration is free, and

deadline for registration is May 15th.

Members of the Network may apply for money to cover travel and accomodation from the Network.

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)

Summer school

on

Nanoscale Materials Physics

Copenhagen August 21 -28, 1994

Nanoscale Materials Physics is one of a series of summer schools initiated by The Danish Research Academy.[1] The school is primarely targeted at PhD students and post-docs, but senior scientist will also be considered. Attendance and acommodation is free and the Danish Research Academy has limited support for travel expenses. The number of participants is limited, and the applicants will be judged on the basis of a short CV and a brief description of their research projects which must be sent to Dr. Hans L. Skriver at the address given below.

Topics:

Atom manipulation, surfaces, interfaces, and layered structures. Growth. Extended defects. Nano-wires. Nano-tribology. Clusters and carbon structures. Experimental techniques and theoretical methods. A single day will be devoted to a *hands on* course in computer simulations of materials properties.

Lecturers:

Lecturers include: F. Besenbacher (Århus), B. Clausen (Topsøe), F. Grey (Tsukuba), K.W. Jacobsen (Lyngby), A.P. Jauho (Lyngby), P. Martin (Stuttgart), B. Persson (Jülich), P. Stoltze (Lyngby), M. Scheffler (Berlin, to be confirmed), D.D. Vvedensky (London).

Place:

The summer school will be held at a conference center 30 km from Copenhagen. The computer simulations will take place at the Technical University of Denmark.

Organization:

Organizing committee: Prof. Jakob Bohr, Prof. Jens K. Nørskov, and Dr. Hans L. Skriver, Technical University of Denmark; Dr. Ivan Stensgaard, University of Aarhus.

Information:

Dr. Hans L. Skriver, CAMP and Physics Department, DTH Bldg 307,
DK-2800 Lyngby.
e-mail: summer@fysik.dth.dk
Phone 45+ 42882488 Ext 3176.

[1]The summer school is fonded by The Danish Research Academy and organized within the Center for Atomic-scale Materials Physics (CAMP) at the Technical University of Denmark and the University of Aarhus.

Subscribers to psik-Network as of March 23, 1994

Belgium

node: Van Doren (Antwerp)
fax: +32 321 80 217

V. Van Doren	vancamp%banruc60@earn-relay.ac.uk
P. Van Camp	vancamp%banruc60@earn-relay.ac.uk

Denmark

node: Christensen (Aarhus)
fax: +45 8612 0740

N. Christensen	nec@dfi.aau.dk
A. Svane	svane@dfi.aau.dk

node: Noerskov (Copenhagen)
fax: +45 459 323 99

K. J. Jacobsen	kwj@fysik.dth.dk
J. Noerskov	NORSKOV@LTF.DTH.DK
J. Noerskov	NORSKOV@FYSIK.DTH.DK
H. Skriver	skriver@fysik.dth.dk

Finland

node: Nieminen (Helsinki)
fax: +385 0457 2302

J. V. Boehm jvboehm@leka.hut.fi
M. J. Puska MJ_PUSKA@HUT.FI
R. Nieminen rniemine@csc.fi

==========

France

==========

node: Boureau (Paris)
fax: +33 1 44 27 62 26

G. Boureau GEB@CCR.JUSSIEU.FR
J. M. Mariott jmma@ccr.jussieu.fr

node: Gautier (Strasbourg)

S. Bouette-Russo sophie@gemme.u-strasbg.fr
H. Dreysse hugues@lugh.u-strasbg.fr
A. Khan ahsan@lugh.u-strasbg.fr
C. Parlebas claude@belenus.u-strasbg.fr
D. STOEFFLER daniel@gemme.u-strasbg.fr

node: Gupta (Orsay)
fax: +33 1 69 855 484

M. Gupta gupta@elstru.isma.u-psud.fr

node: Koenig (Rennes)
fax: +33 99 28 67 17

C. Koenig koenig@univ-rennes1.fr
C. Hoerner hoerner@univ-rennes1.fr

node: Sommers (Orsay)

C. Sommers root@solrt.lps.u-psud.fr

node: Kunc (Paris) ** (not funded)
fax: +33 1 44 27 45 41

K. Kunc kk@ccr.jussieu.fr

node: Pasturel (Grenoble) ** (not funded)

A. Pasturel pasturel@mgstsrv.polycnrs-gre.fr

==========

Germany

==========

node: Andersen (Stuttgart)
fax: +49 711 689 1632

O. K. Andersen andersen@radix2.mpi-stuttgart.mpg.de
Vl. Antonov antonov@radix2.mpi-stuttgart.mpg.de
A. Burkhardt burkhard@radix2.mpi-stuttgart.mpg.de
V. Eyert eyert@radix3.mpi-stuttgart.mpg.de
O. Jepsen jepsen@radix1.mpi-stuttgart.mpg.de
G. Krier krier@radix5.mpi-stuttgart.mpg.de
N. Laouini nozha@radix6.mpi-stuttgart.mpg.de
A. Liechtenstein liechten@radix6.mpi-stuttgart.mpg.de
I. Mazin mazin@radix2.mpi-stuttgart.mpg.de
Z. Szotek dzidka@radix3.mpi-stuttgart.mpg.de
A. Vernes vernes@radix4.mpi-stuttgart.mpg.de

node: Braun (Osnabrueck)
fax: +49 541 969 2670

J. Braun JBRAUN@dosuni1.rz.Uni-Osnabrueck.DE

node: Dederichs (Juelich)
fax: +49 2461 61 2620

S. Bluegel bluegel@iff064.iff.kfa-juelich.de
P. Dederichs IFF140%DJUKFA11@EARN-RELAY.ac.uk
J. Harris IFF068%DJUKFA11@EARN-RELAY.ac.uk
D. Hohl D.HOHL@KFA-JUELICH.DE
L. Nordstrom lars@iff173.iff.kfa-juelich.de
R. Zeller IFF081%DJUKFA11@EARN-RELAY.ac.uk

node: Ebert (Muenich)
fax: +49 89 28 05 248

H. Ebert he@gaia.phys.chemie.uni-muenchen.de

node: Finnis (Stuttgart)
fax: +49 711 22 65 722

M. Finnis finnis@finnis.mpi-stuttgart.mpg.de

node: Kubler (Darmstadt)
fax: +49 6151 163 481

J. Kubler kubler@mad1.fkp.physik.th-darmstadt.de

node: Pollman (Muenster)
fax: +49 251 833 669

J. Pollman POLLMAN@TP2014.UNI-MUENSTER.DE
P. Krueger krueger@tp2018.uni-muenster.de

node: Scheffler (Berlin)
fax: +49 308305531

M. Fuchs fuchs_m@rz-berlin.mpg.de
M. Scheffler scheffler@fhi-berlin.mpg.de

node: Springborg (Konstanz)
fax: +49 7531 88 3898

M. Springborg chwey03@nyx.uni-konstanz.de

node: Winter (Karlsruhe)
fax: +49 7247 824624

R. Schuetz schuetz@infp.kfk.de
H. Winter winter@infp.kfk.de

node: Mertig (Dresden) ** (not funded)

I. Mertig MERTIG@PTPRS2.PHY.TU-DRESDEN.DE

node: Richter (Dresden) ** (not funded)

P. Oppeneer mpag@tudurz.urz.tu-dresden.de
P. Oppeneer peter@tmps06.mpg.tu-dresden.de
M. Richter manuel@tmps06.mpg.tu-dresden.de
L. Steinbeck lutz@tmps06.mpg.tu-dresden.de
P. Ziesche pz@tmps06.mpg.tu-dresden.de

node: Schattke (Kiel) ** (not funded)

W. Schattke SCHATTKE@SOLID.THEO-PHYSIK.UNI-KIEL.D400.DE

==========

Great Britain

==========

node: Gillan (Keele)
fax: +44 782 711093

M. Gillan pha71@seq1.keele.ac.uk
J. Holender pha45@seq1.keele.ac.uk
P. Strange pha05@seq1.keele.ac.uk

node: Gyorffy (Bristol)
fax: +44 272 255 624

E. Bruno pheb@siva.bristol.ac.uk
B. L. Gyorffy blg@siva.bristol.ac.uk

node: Heine (Cambridge)
fax: +44 223 337356

S. Crampin sc10016@phy.cam.ac.uk
V. Heine tcmsec@phx.cam.ac.uk
M. C. Payne mcp1@phy.cam.ac.uk

node: Staunton (Warwick)
fax: +44 203 692 016

J. Staunton phrjz@weedy.warwick.ac.uk

node: Temmerman (Daresbury)
fax: +44 925 603634

P. J. Durham p.j.durham@daresbury.ac.uk
G. Y. Guo G.Y.Guo@daresbury.ac.uk
N. Harrison nh@dl.ac.uk
W. M. Temmerman w.m.temmerman@daresbury.ac.uk

node: Walker (Norwich)
fax: +44 603 585 53

A. Walker a.walker@xgate.uea.ac.uk

node: Paxton (Oxford) ** (not funded)

A. Bratkovski ALEX@BOHR.materials.ox.ac.uk
M. Fearn mike.fearn@materials.ox.ac.uk
C. Goringe GORINGE@BOHR.materials.ox.ac.uk
A. Horsefield ANDREW@BOHR.materials.ox.ac.uk
A. Paxton TONY@NIGHTMARE.materials.ox.ac.uk
D. Pettifor MMLSEC@BOHR.materials.ox.ac.uk
A. Sutton ADRIAN@BOHR.materials.ox.ac.uk

node: Gehring (Sheffield) ** (not funded)
fax: +44 742 728 079

G. Gehring g.gehring@sheffield.ac.uk
T.J. Hammond t.j.hammond@sheffield.ac.uk
M. B. Suvasini m.suvasini@sheffield.ac.uk

==========

Greece

==========

node: Andriotis (Heraklion)
fax: +30 81 239 735

A. Andriotis andriot@iesl.forth.gr

node: Polatoglou (Thessaloniki)
fax: +30 31 20 61 38

H. Polatoglou hariton@donoussa.physics.auth.gr

node: Stefanou (Athens)
fax: +30 172 34100

N. Stefanou nstefan@atlas.uoa.ariadne-t.gr

==========

Ireland

==========

node: Patterson (Dublin)
fax: +353 1 6711 759

D. McDonnaill dmcdonll@tcd.ie
C. Patterson cpttrson@vax1.tcd.ie

==========

Italy

==========

node: Bisi (Trento)
fax: +39 461 88 16 96

O. Bisi bisi@science.unitn.it
E. Lipparini lipparini@itnvax.science.unitn.it

node: Giuliano (Messina)

G. Florio progfin%imeuniv@earn-relay.ac.uk
B. Ginatempo u2ymezh1@cinymp.cineca.it
S. Giuliano giuliano%imeuniv@earn-relay.ac.uk

node: Manghi (Modena)
fax: +39 59 586 011

F. Manghi MANGHI@IMOVX2.UNIMO.IT
S. Ossicini Ossicini@IMOVX2.UNIMO.IT

node: Fiorentini (Cagliari) ** (not funded)

V. Fiorentini fiore@sparc10.unica.it

node: Resta (Trieste) ** (not funded)

S. Baroni baroni@fermi.cm.sissa.it
R. Resta resta@tsmi19.sissa.it

==========

Portugal

==========

node: Martins (Lisbon)
fax: +351 1 52 5843

J. L. Martins jlm@pseudo.inesc.pt

==========

Spain

==========

node: Flores (Madrid)
fax: +34 1 397 4950

F. Flores fernando@uamc10.fmc.uam.es

==========

The Netherlands

==========

node: Kelly (Eindhoven)
fax: +31 40 74 33 65

G. Brocks BROCKS@PRL.PHILIPS.NL
H. Feil FEIL@PRL.PHILIPS.NL
P. Kelly kelly@prl.philips.nl
K. Schep SCHEP@PRL.PHILIPS.NL

node: Inglesfield (Nijmegen)
fax: +31 80 652 120

J. E. Inglesfield johni@sci.kun.nl
M. M. Heinemann martina@sci.kun.nl
J. Thijssen jost@mentor.tvs.kun.nl

==========

Austria

==========

node: Hafner (Vienna)
fax: +43 1 567 760

J. Hafner jhafner@email.tuwien.ac.at

node: Schwarz (Vienna)
fax: +43 1 587 4835

K.-H. Schwarz kschwarz@email.tuwien.ac.at

node: Weinberger (Vienna)
fax: +43 1 587 6199

P. Weinberger pw@eecws4.tuwien.ac.at
J. Kudrnovsky e158wdah@awiuni11.edvz.univie.ac.at

==========

Switzerland

==========

node: Bloechl (Zurich)
fax: +41 1 724 0809

P. Bloechl BLO@ZURICH.IBM.COM

node: Baratoff (Basel) ** (not funded)

A. Baratoff baratoff@urz.unibas.ch

node: Car (Lausanne) ** (not funded)
fax: +41 22 781 21 92

N. Binggeli binggeli@eldp.epfl.ch
R. Car car@eldp.epfl.ch
G. Galli galli@eldp.epfl.ch
F. Gygi gygi@eldp.epfl.ch

==========

Sweden

==========

node: Eriksson (Upsala) ** (not funded)

O. Eriksson olle@lina.fysik.uu.se

==========

Czech Republic

==========

node: Sob (Brno) ** (not funded)
fax: +42 5 412 123 01

V. Drchal drchal@fzu.cz
M. Sob sob@elanor.sci.muni.cs
M. Sob mojmir@drs.ipm.cs
I. Turek turek@ipm.cz

==========

Poland

==========

node: Kiejna (Wroclaw) ** (not funded)
fax: +48 71 214 454

A. Kiejna	KIEJNA%PLWRUW11.earn@earn-relay.ac.uk
A. Rubaszek	intmet%plwrtu11.earn@earn-relay.ac.uk

==========

Russia

==========

node: Kulikov (Moscow) ** (not funded)

N.I. Kulikov	hpp@adonis.iasnet.com
M.V. Magnitskaya	hpp@adonis.iasnet.com
A.F. Tatarchenko	hpp@adonis.iasnet.com

node: Maksimov (Moscow) ** (not funded)
fax: +7 095 135 85 33

O. Ivanov	ivanov@td.fian.free.net
E. Kulatov	kulatov@smp.gpi.msk.su
E.G. Maksimov	maksimov@td.fian.free.net
A. Nargizyan	nargizyan@td.fian.free.net
D. Savrasov	savrasow@td.fian.free.net
S. Savrasov	savrasov@td.fian.free.net
Yu. Uspenskii	uspenskii@td.fian.free.net

==========

Parties interested to receive all Network's e-mail messages

==========

Australia

==========

M. Radny	phmwr@cc.newcastle.edu.au

==========

United States of America

==========

W. Hierse	wghiers@cs.sandia.gov

==========

Embedding muffin-tins into a finite difference grid.

J.M. Thijssen and J.E. Inglesfield .
Department of Physics, University of Nijmegen
Toernooiveld, NL-6525 ED Nijmegen

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.

(submitted to Physical Review B, February 1994)
The REVTEX version can be obtained from jost@tvs.kun.nl

Calculated Crystal Field Parameters for Rare Earth Impurities in Noble Metals.

Lutz Steinbeck, Manuel Richter, Helmut Eschrig
Max-Planck-Research-Group "Electron Systems", Department of Physics,
University of Technology, Mommsenstr. 13, D-01062 Dresden, Germany
Ulrike Nitzsche
Institute of Theoretical Physics, Department of Physics,
University of Technology, Mommsenstr. 13, D-01062 Dresden, Germany

Abstract

From first-principles density functional calculations of the charge distribution the crystal-field (CF) parameters for 4f states of Er and Dy impurities in Ag and Au have been evaluated. The calculations are based on an optimized LCAO scheme, where the local density approximation (LDA) is used for the conduction electron states while the localized rare earth 4f states are treated as 'open core shell'. As the 4f localization cannot be properly described within LDA, self-interaction correction for the 4f states is included. In this way, any artificial constraints on the 4f charge density employed in earlier first-principles CF calculations are avoided. The calculated CF parameters agree well with recent neutron scattering data.

(accepted for publication in Phys. Rev. B)

The REVTEX version can be obtained from lutz@tmps06.mpg.tu-dresden.de

ELECTRONIC STRUCTURE AND HYBRIDIZATION IN U_2T_2In (T = Co, Ni, Pd) INTERMETALLICS.

M. Diviš,
Department of Metal Physics, Charles University, Ke Karlovu 5,
121 16 Prague 2, Czech Republic

M. Richter and H. Eschrig
MPG Research Group 'Electron Systems', University of Technology,
D-01062 Dresden, Germany

Abstract

Ab initio electronic structure calculations of U_2T_2In (T = Co, Ni, Pd) intermetallic compounds were performed using an optimized LCAO method based on the LDA approximation. The particular electronic structure and related properties of U_2T_2In originate from the interplay between the band filling of the free electron background (s-, p- and uranium d-electrons), transition metal bonding bands and covalency (hybridization) between bonding predominantly d-states of T atoms and antibonding predominantly f-states of U atoms. The observed experimental trends in the term γT and magnetic properties of U_2T_2In are qualitatively consistent with the results of our approach.

(accepted for publication in Solid State Communications)

The LATEX version (without figures) or a hardcopy can be obtained from
manuel@tmps06.mpg.tu-dresden.de

Gap opening in Si ultra-thin layers: role of confined and interface states

Stefano Ossicini, A. Fasolino, F. Bernardini
Dipartimento di Fisica, Università di Modena,
Via Campi 213/A, 41100 Modena, Italy

Abstract

We present first principle calculations of ultra-thin silicon (111) layers embedded in CaF_2, a lattice matched insulator. Our all electron calculation allows to check the quantum confinement hypothesis for the Si band gap opening as a function of thickness. We find that the gap opening is mostly due to the valence band while the lowest conduction band states shift very modestly due to their pronounced interface character. The latter states are very sensitive to the sample design. We suggest that a quasi direct band gap can be achieved by stacking Si layers of different thickness.

(to appear in Phys. Rev. Lett., February 14, 1994)
The REVTEX version can be obtained from ossicini@imovx2.unimo.it

Ab Initio Calculation of Quantum Well States in Cu/Co (100)

L. Nordström, P. Lang, R. Zeller, and P.H. Dederichs
Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

Abstract

A first principle calculation of spin polarized quantum well states within Cu/Co has been performed using a KKR-Green's function method. Results for up to 25 ML Cu and several ML Co are presented, which are in very good agreement with experiments. In addition an important new effect is found arising from the resonant interaction of QW states with size-quantized *d*-states of the Co layers. This effect leads to branch jumps in the dispersion of the QW states and to a strong reduction of their confinement.

(Submitted to Phys. Rev. Lett.)
The REVTEX manuscript can be obtained from lars@iff173.iff.kfa-juelich.de

The Electronic Structures of CeNiSn, CePdSn and CePtSn

T. J. Hammond, G. A. Gehring, M. B. Suvasini
Physics Department, University of Sheffield, Sheffield, S3 7RH, UK
W. M. Temmerman
SERC Daresbury Laboratory, Warrington, WA4 4AD, UK

Abstract

We have performed self-consistent, first principles band structure calculations on the isostructural heavy fermion materials CeNiSn, CePdSn and CePtSn. CeNiSn behaves as a heavy fermion compound down to 7K where a small, anisotropic energy gap develops. In contrast CePdSn and CePtSn have magnetic, metallic ground states, both with $T_N = 7.5$K. Our calculations reveal band structures in good agreement with the experimental observations. We find an insulating band structure for CeNiSn which displays no tendency to form a magnetic ground state. We interpret this to mean that the energy gap may be due to hybridisation. For CePdSn and CePtSn we find metallic ground states and spin-polarised calculations reveal the existence of a stable magnetic state for CePdSn with a moment of $0.84\mu_B$ per cerium atom, whilst for CePtSn a magnetic state is only obtained when the lattice is expanded.

(Submitted to Phys. Rev. B.)
The REVTEX manuscript can be obtained from T.J.Hammond@sheffield.ac.uk

Breathing instability and disproportionation of Bi $^{4+}$ ions in $BaBiO_3$

I.I. Mazin and A.I. Liechtenstein
Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1,
D-70569 Stuttgart, FRG.
O.V Ivanov
P.N. Lebedev Physical Institute, Leninski 53, 117924 Moscow, Russia

Abstract

We discuss the origin of the so-called breathing instability of the $BaBiO_3$ perovskite in view of the, seemingly contradictory, results of the full-potential LDA calculations and the quasi-ionic (Potential-Induced Breathing, PIB) calculations. We demonstrate that both sets of results are in fact not in contradiction with, but rather complement, each other. In particular, a proper comparison of the LMTO and PIB calculations shows, to what extent the breathing instability is driven by the tendency of the Bi^{4+} ions to disproportionate into Bi^{3+}+Bi^{5+} (more correctly, into Bi^{4-x}+Bi^{4+x}), as had been suggested by some authors, and to what extent by the opening of the gap in Peierls' spirit.

Talk presented in the 3rd Williamsburg Conference on First-Principle calculations in Ferroelectrics, to be published in *Ferroelectrics*
The REVTEX manuscript can be obtained from mazin@radix2.mpi-stuttgart.mpg.de

Three-molecular-orbital treatment of the orientational ordering in A_3C_{60}

I. I. Mazin, A. I. Liechtenstein, O. Gunnarsson, and O. K. Andersen
Max-Planck-Institut für Festkörperforschung,
P.O.B. 800665, D-70506 Stuttgart, F.R.G.

Abstract

We have analyzed the band energy of the t_{1u} band of A_3C_{60}, using the three-molecular-orbital tight-binding model. It turns out that this energy can with a good accuracy be described by the antiferromagnetic Ising model, where the two allowed orientations of each molecule play the role of the two spin directions. We also show that such a description is limited to disordered and short-range ordered structures, while the long-range ordered structures are affected by the band-structure effects leading to peaks in the density of states.

submitted to Solid State Commun.
The REVTEX manuscript can be obtained from mazin@radix2.mpi-stuttgart.mpg.de

Momentum dependence of the linewidth of Raman-active phonons in the normal state of $YBa_2Cu_3O_7$.

O.Jepsen, I.I.Mazin, A.I.Liechtenstein, O.K.Andersen
Max-Planck-Institut für Festkörperforschung, Stuttgart, F.R.G.

Abstract

In view of recent experimental measurements of the wave vector dependence of the phonon linewidth for near-zone-center Raman phonons, we have refined our previous frozen-phonon calculations of this quantity, now on an expanded q-scale and with higher accuracy. These new results allow for a quantitative comparison of the LDA prediction with the experiment. In particular, the thresholds for the Landau damping of the Raman phonons agree very well with the experiment, demonstrating that the LDA Fermi velocities are correct. There is, however, a systematic underestimation of the linewidth. A possible reason for that is that the magnitude of the damping depens not only on the electronic velocities, but also on masses, which may be subject to a much stronger renormalization.

to be submitted
Available on request from Igor Mazin, MAZIN AT RADIX2.MPI-STUTTGART.MPG.DE

Displacive excitation of coherent phonons in $YBa_2Cu_3O_7$

I. I. Mazin*, A. I. Liechtenstein. O. Jepsen,
O. K. Andersen, and C. O. Rodriguez
Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1,
D-70569 Stuttgart, FRG.

Abstract

We suggest a microscopic model that provides a consistent explanation of the recent femtosecond pump-probe experiments on $YBa_2Cu_3O_7$, including the fact that the reflectivity change in the superconducting state is much larger than that in the normal state. In this model, not only the oscillatory part of the reflectivity, but also the total reflectivity change, is due to displacive excitation of coherent phonons. The microscopic reason for this excitation is that superconductivity induces small displacements in the equilibrium positions of the ions, since the pairing energy depends on the density of states at the Fermi level, which changes with the ionic positions. When superconductivity is destroyed by the femtosecond laser pulse, the ions are pulled back to their normal equilibrium positions, thus exciting coherent phonons. The relative size of the oscillatory contribution to the reflectivity depends upon the ratio of the phonon period to the time scale of the pair breaking, and when this ratio is small, the oscillations are suppressed, as observed in the experiment. *Ab initio* calculations confirm this model. The model also provides an explanation why the magnitude of the 150 cm^{-1} mode below T_c may be much smaller than that of the 120 cm^{-1} mode.

to be published in PRB on April 1, 1994
*mazin@radix2.mpi-stuttgart.mpg.de