HCM Newsletter

Ψ_k Network

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

Number 8 April 1995

Editor: Z. (Dzidka) Szotek
Proposal: ERB4050PL930589
Contract: ERBCHRXCT930369

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Editorial

In this Newsletter, as usually, the abstracts are placed at the end, before the **Highlight of the Month Section**, containing *O. Bisi's* (University of Trento) comment on **'Porous Silicon'**. Straight after the editorial we have enumerated until now *'non-funded'* nodes that participate in the enlargement of the Network.
In the section **News from the Network** we have given a summary of the main issues discussed by the *Network's Management Board* at the 4th March meeting in Paris. This is followed by the **1st circular** of the *Network's big Conference*, to be held in Schwäbisch Gmünd (Germany) on 18-21 September 1996, and the **2nd circular** of the *ERC Conference*, to be held in Lunteren (The Netherlands) on 9-14 September 1995. In the section **News from the Working Groups** you will find reports on collaborative visits and/or workshops. Straight after the reports you can find **2nd announcement of the Hands-on Workshop for FP-LAPW-Wien95 code**, and an **announcement of the available Ph. D studentships at the University of London**. Additionaly, there is an informatin on the **Electronic Structure Network in Argentina** which could be of interest to all of us.

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

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

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

This also contains pointers to two other nodes: *O.K. Andersen (Stuttgart)* which includes information on the **Network Conference**, and *J. Nørskov (Lyngby)* with information on CAMP. If you mantain a home page on your activities we will be happy to include a pointer from the *Network's* home page to your home page.

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

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

Network Enlargement

Following our call in the February issue of the *Newsletter*, concerning the enlargement of the *Network* within the present contract, the following twenty groups expressed interest in being included into the *Network* as funded nodes:

P. Bruno *(CNRS, Orsay, France)*
S. Crampin *(Bath, UK)*
O. Eriksson *(Uppsala, Sweden)*
M. Finnis *(Belfast, UK)*
F. Fiorentini *(Cagliari, Italy)*
G. Gehring *(Sheffield, UK)*
E.K.U. Gross *(Würzburg, Germany)*
F. Gygi *(IRRMA, Lausanne, Switzerland)*
W. Hergert *(Halle, Germany)*
J.E. Inglesfield *(Cardiff, UK)*
K. Kunc *(CNRS, Paris, France)*
I. Mertig *(Dresden, Germany)*
M. Methfessel *Frankfurt/O, Germany)*
R. Monnier *(ETH, Zürich, Switzerland)*
N.I. Papanikolaou *(Ioannina, Greece)*
A. Pasturel *(CNRS, Grenoble, France)*
A. Paxton *(Oxford, UK)*
M. Richter *(UT, Dresden, Germany)*
E. Sandré *(CNRS, Grenoble, France)*
C.M.J. Wijers *(Twente, The Netherlands)*

Please note that the above list of nodes has been forwarded to the Commission in Brussels with request of including them into the present contract with the status of 'a funded node'. There will be no further expansions of the *Network* beyond this. The members of the above nodes, with the exception of Switzerland and Sweden (since we are still operating within the Framework III), will now be able to claim *Network's* money for participating in the Network's activities.

News from the Network

At the last *Network's Management Board* meeting in Paris on March 4, 1995 two important issues were discussed. Firstly, the **1st circular** and the timetable of the big conference of the *Network*, to be held in Schwäbisch Gmünd in September 1996, were discussed and agreed. Secondly, the Board discussed the strategy and projects for the renewal of the *Network* within the **Framework IV** of the European Union Commission.

Conference:
With respect to the **1st circular** of the *Network's Conference* you can find details on the next four pages. This information is also available on the WWW by accessing the Stuttgart home page referring to both the *Conference* and the *Network*:

http://radix2.mpi-stuttgart.mpg.de

Funding:
Regarding funding for continuing the *Network's* activity beyond 1996, the *NMB* decided to apply for financial support to the **European Science Fundation**, believing that our present Network is not focused enough in terms of the new Framework IV of the EU Commission, to be able to continue in its present form. However, the coordinator is going to explore further possibilities for our *Network* in direct discussions with the Commission in Brussels.

Acknowledging the Network:

The NMB agreed that it is very important for the renewal of the Network to acknowledge the Network in all our publications that have benefited from collaborations within the Network, even if the Network funds have not actually been used. This also refers to cases where a publication has benefited from a computer code picked up at various workshops, organised by the Network, or even straight from a member of the Network. We need to stress the collaborations that exist within the Network. The following formula could be used in the acknowledgement:

This work has benefited from collaborations within, and has been partially funded by, the Network on "Ab-initio (from electronic structure) calculation of complex processes in materials" (contract: ERBCHRXCT930369).

If the Network's funds have not been used, then the part of the sentence:
...", and was partially funded by," ... should be omitted.

First Circular: ψ_k-Conference

organised by

European Union HCM Network

"Ab-initio (from electronic structure) calculation of complex processes in materials"

Schwäbisch Gmünd, September 18-21, 1996

Conference Chairman: Professor O.K. Andersen

Please note that this circular is distributed only via electronic mail and is also available on: **http://radix2.mpi-stuttgart.mpg.de**!

Main Topics of the Conference:

- Density Functional Molecular Dynamics Simulation: methods and applications
- New Developments in Muffin-tin and Pseudopotential Techniques
- Quantum Monte Carlo Calculations
- Beyond the Local Density Approximation
- Solving the Bogolubov de Gennes Equations
- Quasiparticles
- Approximate Methods for Large Systems
- Parallel Algorithms (Parallelisation)
- Applications to all aspects of Condensed Matter and Materials Science:

  Electron spectroscopies
  Novel superconductors
  Magnetic multilayers
  Oxides/metal interfaces
  Reactions at surfaces
  Semiconductor heterostructures and quantum wires
  Carbon structures
  Molecular materials

- **Participation:**

- The conference is open to anyone interested.
- Expected attendance:300.
- Every abstract will be accepted, either as a contributed talk or as a poster, subject to the limitation that each participant presents at most one talk or poster.

- **Timetable:**

March 1995	First Circular
November 1995	Second Circular including Suggestion Forms for Symposia and Invited Speakers
February 1996	Deadline for Suggestions
April 1996	Third Circular including Details about Symposia and Invited Speakers
May 1996	Deadline for Submission of Abstracts and Registration
June 1996	Final Programme
September 1996	Conference

- **Contact addresses and further information:**

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- FAX: +49-711-689 1632
- Mail:
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  Max-Planck-Institut für Festkörperforschung
  Postfach 80 06 65
  D-70506 Stuttgart
  Germany

- **Location:**

Schwäbisch Gmünd is located in south-west Germany, 50 km east of Stuttgart, the capital city of the state of Baden-Württemberg (B-W). It is easily accesible by public transportation from Stuttgart. The Stuttgart International Airport is located 15 km south of the city centre.
The conference will be held at the Stadtgarten in Schwäbisch Gmünd, one of B-W's most modern conference centres. The Stadtgarten is located in the centre of town, within walking distance from most of the hotel accomodation. Schwäbisch Gmünd is a lovly old town with a population of 60000 and with a history dating back to the Roman Empire in the 2nd century. In the 12th century it became the first of several imperial towns founded by the Hohenstaufen dynasty to protect their empire. Many original old buildings show the transition of the former Free Imperial City from Gothic through to Renaissance to Baroque, and the coexistence of 19th century palatal grandeur with contemporary architecture.

A schematic map of the location of Schwäbisch Gmünd is printed on the following page, and a nice coloured picture of the town can be found on O.K. Andersen's WWW home page: http://radix2.mpi-stuttgart.mpg.de.

- **Cost and financial support:**

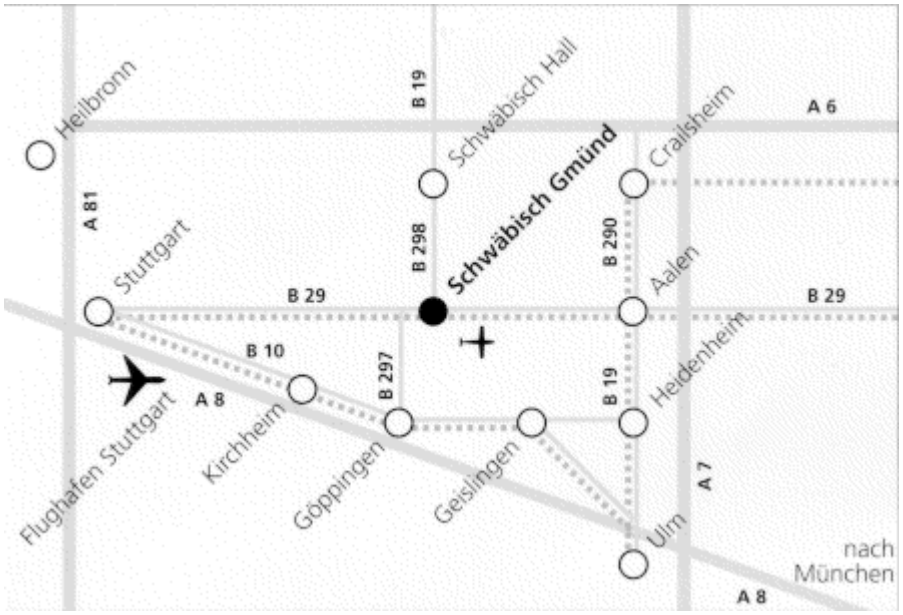
The estimated minimum total cost of attending the Conference will be ∼500 ECU (including travel and living expenses).

EU Members:
There will be some Network grants available for attending the conference, and priority will be given to young scientists (PhD students, postdocs, etc.); exclusively EU nationals and members of the Network, but details still need to be worked out and will be announced later on.

Eastern Europeans:
The organisers will seek additional funds to support the participation of scientists from Eastern and Central European countries. However, since these funds will probably be very modest, therefore those scientists from Eastern and Central Europe who would need financial support to attend the Conference should contact Professor Ole Krogh Andersen a.s.a.p. on:

psik@radix2.mpi-stuttgart.mpg.de.

Conference Location: Schwäbisch Gmünd (Germany)



EUROPEAN RESEARCH CONFERENCES

2nd Circular

RESEARCH CONFERENCES ON

ELECTRONIC STRUCTURE OF SOLIDS:

Itinerant Magnetism

Lunteren, The Netherlands, 9-14 September 1995

(*Co-sponsored by the European Science Foundation and The Euroconferences Activity of the European Union*)

Chairman: Professor Balazs L. Gyorffy (Bristol),
Vice-chairman: Dr. Peter Blöchl (Zürich)

This is our 4th Euro Research Conference on the Computational Physics of the Electronic Structure in Solids. The previous ones emphasised: The Computational Leading Edge (Cambridge 1992), Surfaces and Interfaces (Porto Carras 1993), Dynamics and Excitations (Gausdal 1994). In 1995 we shall focus on the **first-principles description of magnetic phenomena in solids**. While contributions to all subjects which answer the above broad description will be welcomed we have selected the following topics for special emphasis:

- Spin-Polarised Band Theory (Orbital Magnetism, Heavy Fermions, Spin Fluctuations, etc.)
- Magnetism at Surfaces and Interfaces (Perpendicular Magnetism, Exchange Anisotropy, etc.)
- Magnetic Metallic Multilayers (Oscillatory Coupling, Giant Magneto-resistance, etc.)
- Magnetism in Disordered Systems (Spin Glasses, Metallic Glasses, Magnetic Alloys, etc.)
- Density Functional Theory and Model Hamiltonians (LDA+U, etc.)

The speakers will include:

W.M. Temmerman (Daresbury)
P. Fulde (Dresden)
H. Skriver (Lyngby)
W.E. Piskett (Washington)
B. Johansson (Uppsala)
A.M. Oleś (Cracow)
H. Ebert (München)
P.A. Lingård (Risø)
P. Dederichs (Jülich)
L. Szunyogh (Budapest)
S. Blügel (Jülich)
I. Mertig (Dresden)
F. Gautier (Strasbourg)
J.B. Staunton (Warwick)
J. Kudrnovský (Prague)
R.A. de Groot (Nijmegen)
P. Entel (Duisburg)
J. Hafner (Vienna)
F. Aryasetiawan (Lund)
J. Mathon (London)
P. Kelly (Eindhoven)

Suggestions: The program is not yet complete and the organisers welcome suggestions for invited speakers which can be submitted to Professor B.L. Gyorffy (blg@siva.bristol.ac.uk).

Posters: All participants will be encouraged to present posters.

Financial Assistance: A limited budget exists to support qualified students and postdocs. Applications should include C.V., a brief resumé of current research and names of two referees.

Enquiries: Further information is available from the Conference Chairman Professor B.L. Gyorffy (blg@siva.bristol.ac.uk) or the Secretary Dr. Stefan Blügel (s.bluegel@kfa-juelich.de) or from secretariat.

News from the Working Groups

Report on
"Solving the Bogoliubov-de Gennes Equations for Superconductors"

Two-Day Workshop (29-30 October 1994) at University of Bristol, U.K.
organized by CCP9 (Electronic Structure of Solids) and HCM Psik-Network

In general solving the BdG equations allows one to go beyond the simple BCS model. This meeting reviewed the application of BdG equations in a variety of systems such as the high T_c materials, mesoscopic systems, magnetic multilayers, negative U Hubbard model, $NbSe_2$, charged Bose gas. The relativistic extension was discussed. Exciting new developments include the use of the BdG equations in analysis of the de Haas-van Alphen oscillations in the superconducting state as a method to obtain the k-dependent superconducting gap.

The programme of this meeting was:

Annett JF	"D-wave pairing in high Tc Superconductors"
Temmerman WM	"The Quasi-Particle Spectrum of Bilayer Materials"
Guo GY	"De Haas-van Alphen Oscillations in Superconducting NbSe2"
Miller P	"De Haas-van Alphen oscillations in the Superconducting State"
Tavern S	"Superfluidity in a Two Dimensional Negative U Hubbard Model"
Capelle K	"The Relativistic Bogoliubov-de Gennes Equation"
Sipr O	"Magnetic Coupling between Metallic Multilayers across Superconducting Spacers"
Martin A	"Self-Consistent Solutions of the BdG Equation for Mesoscopic Structures"
Litak G	"A Recursion Method for solving the Bogoliubov-de Gennes Equation"
Wilson J	"The symmetry of the Superconducting Gap"
Leadbeater M	"Superconducting Analogues of the Aharanov-Bohm-Casher Effect"
Alexandrov AS	"The Bogoliubov-de Gennes Equations for a Charged Bose Gas""
Gyorffy BL	"Disordered Local Pairing"

The were over twenty participants and among them: J.F. Annett, P. Miller, B.L. Gyorffy, S. Tavern, J. Wilson, S. Hayden (Bristol); O. Sipr (Prague); B. Ujfalussy (Budapest); G. Litak (Lublin); K. Capelle (Würtzburg); W.M. Temmerman, Z. Szotek, G.Y. Guo (Daresbury); H. Winter (Karlsruhe); A. Martin, M. Leadbeater (Lancaster); A.S. Alexandrov (Cambridge)

(Walter Temmerman)

Report on the Collaborative Visit of C. Sommers (Paris) to Vienna, 15-19th January 1995

Ingrid Mertig and myself met with Peter Weinberger and Peter Levy in Vienna.

The ideas we explored were on the scattering of conduction electrons by impurities and by interface roughness in multilayered structures. Essentially we want to update the work of Mertig et al. (MRS Sym. Proc. **253** (1992) 249) which is the scattering by impurities in ferromagnetic alloys to magnetic multilayers, i.e. in layered structures the scattering will depend on the position of the impurity relative to the interfaces and the magnetic configuration of the multilayer. The posibilites we considered were one interface, i.e. two semi-infinite layers to see how the scattering by an impurity varies as it approaches the interface. With one interface done we could proceed to 2,3 and a periodic superlattice.

The scattering at interfaces should probably be dealt with by CPAing the two monolayers adjacent to the interface.

In general we discussed the feasability of *ab-initio* calculations of electrical transport of transition layer multilayers. Under discussion were to see which computer codes already existed and which would be needed for these types of materials.

In particular we wanted to determine what part of existing codes for determining the interlayer magnetic coupling could be used for the transport calculations. At the end of the meeting the broad outline of what additional codes to be written were determined.

I wish to be reimboursed for the plane fare Paris-Vienna 1877 FF and 5 days subsistance at 40 ECU/day = 240 ECU

(Charles Sommers)

Report on the Collaborative Visit of I. Mertig (Dresden) to Vienna, 17-18th January 1995

Peter Weinberger, Charles Sommers, Peter Levy, Joseph Kudrnovsy, Vaclav Drchal and myself discussed at a miniworkshop the problems concerning *ab-initio* calculations of giant magnetoresistance (GMR) in magnetic multilayers.

Starting from our results on the GMR of Fe/Cr/Fe superlattices (P.Zahn, I.M., M.Richter and H.Eschrig,to be published) which consider the influence of spin-dependent scattering due to bulk impurities in a ferromagnetic host material (I.M., R.Zeller and P.H.Dederichs, Phys. Rev. B**47**, 16178 (1993)) we discussed the possibilities of an *ab-initio* calculation taking into account surface roughness.

One way to describe interface roughness is to simulate an interface alloy. The interface alloy should be dealt with an CPA prescription.

The main point of the discussion was the calculation of the transport properties for a layerd system including disordered interface layers.

I wish to be reimboursed for the train fare Dresden-Vienna at 270 DM and 2 days subsistance at 40 ECU/day = 80 ECU

(I. Mertig)

Report on the Collaborative Visit of J.E. Inglesfield, M. Heinemann and J. van Hoof (Nijmegen) to the group of R. Podloucky, Vienna, 26-30th January 1995

The aim of this visit was to discuss LAPW programs for surface calculations - the embedding techniques being developed in Nijmegen compared with the slab studies being carried out in Vienna by the group of Raimund Podloucky. One useful point of discussion, particularly relevant to ionic systems, was the electrostatic boundary condition applied to the solution of Poisson's equation in an embedded slab, as well as the embedding potential itself for the solution of the Schroedinger equation. The lack of precise charge neutrality in the embedded slab was also discussed.

We hope to collaborate in the near future on a comparison of embedding versus slabs with a study of real systems. Particular efforts are planned for an embedding scheme which includes energetics and forces.

(John Inglesfield)

Report on the Collaborative Visit of S. Simak (Rennes) to the Max-Plank Institut, Stuttgart, Germany, 6-7 February, 1995

A collaborative visit to Stuttgart was devoted to work with the last version of the TB-LMTO program of Professor Andersen's group in order to use it for self-consistent calculations of the electronic structure of molecular crystals. The problem which should be solved is structural instabilities in such crystals: dimerizations etc. For two days of my visit
1) I learned to work with the program;
2) A number of test-calculations were done. Since molecular crystals have complicated structures, it is necessary to take into account a lot of empty spheres (ES). The problem of how many ES are required and how to decide the positions for such spheres in the unit sell is not trivial. But the program solves it. It took more than 50 ES for $TTF - 2.5Cl_2BQ$ crystal. Calculated band structure looks reasonable.
So it was a useful visit and its results can help me to solve the problem which I have.
The amount I had received from the network for the travel (train: economic class) and per-diem subsistance almost covered my expenses.

(Sergei Simak)

Report on a visit by K. Capelle (Würzburg) to Bristol

From 24 February to 4 March, I was at the H.H. Willis Laboratory in Bristol to work with B.L. Gyorffy on dichroism in superconductors. The visit was funded by Ψ_k-Network.

We discussed relativistic effects in superconductors in general and dichroism in superconductors in particular. From the theory of relativistic effects in superconductors, developed by the Würzburg group, I had derived a general formula for dichroism in superconductors using a method suggested to me by B.L. Gyorffy during a previous visit of mine in Bristol. We now had several interesting discussions about this formula and its implications. We also discussed the Bogolubov-de Gennes equations and their various applications and generalizations.

To study the effect of spin-orbit coupling on dichroism in superconductors we then looked at a number of simple model systems where one can obtain analytical results. We verified that the formula does not predict dichroism for systems which do not break time-reversal and inversion symmetry.

For systems which do break these symmetries, the theory predicts dichroism in superconductors from two sources, diagonal and off-diagonal spin-orbit coupling. We discussed systems where these effects can be seen and how to solve the equations for these cases.

(Klaus Capelle)

2nd Announcement

HCM WORKSHOP

Full-Potential LAPW calculations with the WIEN95 code

April 19-22, 1995
Technical University Vienna, Austria
Chairman: K. Schwarz
Sponsors:
Human Capital and Mobility Programme
Austrian Science Foundation (FWF)
Bank Austria
Creditanstalt Bankverein

The new version of the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the WIEN95 code has been developed and improved with the help of many users, especially in collaboration with the groups:

Technical University Vienna Fritz-Haber Institute (Berlin)
Max-Planck-Institut f. Metallforschung (Stuttgart)
Universitaet Graz

General Information

Conference site:
The conference will take place at the Technical University of Vienna, A-1040 Wien, Wiedner Hauptstr.8-10. This university buildung (entrance Resselgasse) is light green and has three towers (red, yellow and green section). Registration and lectures are on second floor (HS 8: Noebauer) yellow tower. The computer room (for exercises) is next to it.

Registration:
Tuesday, April 19, 1995 at 5 - 7 pm.
Location: second floor Freihaus (yellow tower, see above). Welcome reception (light refreshments) starting at 6 pm at the registration.

Social events:

"Heuriger", Friday, 21 April 1995.

An informal evening with a dinner (a selection of traditional Heurigen delicacies) and local wines at "Buschenschak Wilfinger", Neustift am Wald, 1190 Wien, Hameaustr. 5. Departure by bus at 6 pm from conference site (Resselgasse/Operngasse). Bus will return by 11 pm.

Price per person: ATS 350 (accompaning persons are welcome). Please, register and pay for the "Heuriger" before Wednesday 2 pm.

Scientific Programme

Wednesday, April 19, 1995 *T. Butz*

8.00 Registration

9.00 K.Schwarz (TU Wien):
Density functional theory and the concepts of
the linarized augmented plane wave (LAPW) method

10.00 P.Blaha (TU Wien):
An overview of the new WIEN95 package

11.00 Coffee break

11.30 Exercise I (getting started, struct file, init)

13.00 Lunch (Mensa)

14.00 P.Blaha (TU Wien):
WIEN95: input and output files

15.00 Exercise II (run first examples)

Thursday, April 20, 1995 *C. Ambrosch*

9.00 P.Dufek (TU Wien):
The use of local orbitals

10.00 P.Blaha (TU Wien):
WIEN95: analyze results (charges, densities, density of states)

11.00 Coffee break

11.30 Exercise III (run first examples)

13.00 Lunch (Mensa)

14.00 K.Schwarz (TU Wien):
Results with the generalized gradient approximation (GGA)

15.00 Exercise IV (run and analyze test cases)

Friday, April 21, 1995 *K. Schwarz*

9.00 M.Faehnle (MPI Metallforschung, Stuttgart):
Different approaches to ab-initio forces

10.00 B.Kohler (Fritz-Haber Institute der MPG, Berlin):
Force calculations according to Yu-Singh-Krakauer:
application to molecules and surfaces, geometry optimizers

11.00 Coffee break

11.30 H.Krimmel (MPI Metallforschung, Stuttgart):
Calculation of atomic forces according to FLAPW (Soler-Williams)

12.10 General discussion on future of WIEN95
(new features, newsletter, communication, exchange of ideas, etc)

13.00 Lunch (Mensa)

14.00 Short POSTER presentation:
2 minutes (2 transparancies) per poster

14.45 POSTER session

18.00 Departure for "Heuriger" (Viennese wine tavern)

Saturday, April 22, 1995 *M. Faehnle*

9.00 C.Ambrosch-Draxl (Univ.Graz):
Optical properties by means of LDA band structure calculations

9.45 E.Deiss (Paul Scherrer Inst.):
Modeling of lithium intercalation into electrode materials

10.10 P.Novak (Inst.of.Physics, Praha):
RE compounds - calculation of crystal field parameters and
anisotropic exchange using LAPW

10.35 Coffee break

11.00 G.Nunes (INESC, Lisboa):
Pseudopotentials for calculations and simulations

11.25 B.Winkler (Univ.Kiel):
Applications in mineralogy

11.50 G.Botton (Cambride):
Electron energy loss spectroscopy to study the bond in materials:
experiments and theory

12.15 Lunch (in nearby restaurants)

14.00 Exercise V (gain experience)

Posters:

Poster size: width 100 cm, height 200 cm.

R.Abt and C.Ambrosch-Draxl (Univ.Graz): 'Optical properties by the LAPW code WIEN95: from Si to high temperature superconductors'.

P.Alippi and M.Scheffler (Fritz-Haber Institute der MPG, Berlin): 'Study of metastable metallic phases: FLAPW calculations on Cu and comparison with other methods'.

L.Benco (Slovak Acad.Science, Bratislava): 'The electronic structure of the grain boundary of beta-Si_3N_4'.

A.Delin, L.Fast, O.Eriksson, and B.Johansson (Univ. Uppsala): 'Calculated equilibrium properties of the lanthanides: an LDA-GGA comparison'.

R.Holmestad, J.M.Zuo, J.A.Henderson, and R.Hioer (U.Trondheim): 'Charge density in TiAl intermetallics'.

C.Holtfort (U.Duisburg): 'Total energy calculations for transition metal hydrides (ZrH_2) in cubic and tetragonal structures'.

I.A.Abrikosov, O.Eriksson, P.Soderlind, P.James, H.L.Skriver, and B.Johansson (U.Uppsala): 'Theoretical aspects of FeNi Invar alloys'.

R.Kouba and C.Ambrosch-Draxl (Univ.Graz): 'Atomic forces within the WIEN-code: a detailed convergence study for selected phonon modes'.

E.Kunoff (Ben-Gurion Univ.): 'Electric field gradients in H-doped $YBa_2Cu_3O_{7-x}$'.

F.Maca (Czech Academy of Sciences, Praha): 'Electronic structure of p(2x2)Na on Al(111) and STM images via FPLAPW'.

S.Matar (CNRS Bordeaux): 'Investigation of the electronic and magnetic structures of U_2T_2Sn ((T=Fe,Co,Ni) stannides '.

G.Nunes (Lisboa): 'Cl and Ag pseudopotentials for AgCl/Cl simulations'.

J.Scheipers and W.Schirmacher (TU Munich): 'Self-Consistent theory of phonon damping due to anharmonic effects'.

A.Schirmer and P.Heitjans (U.Hannover): 'Electric field gradients in lithium-graphite intercalation compounds: Experimental results and planned calculations'.

For further information contact the organizer:

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Getreidemarkt 9/158
A-1060 Vienna Austria
Email: kschwarz@email.tuwien.ac.at
Fax: +43 (1) 5868 937

Announcement: Ph. D Studentships

Physics Department, Queen Mary and Westfield College,
University of London

There are two postgraduate studentships available for those who would like to do a Ph. D in solid state computational physics.

The active areas of research include the calculation of the band structures, pressures and susceptibilities of complex solids from first principles band structures. Our group have already developed suites of programs using LMTO bands which run on a range of parallel computers. We are in the process of extending our codes to calculate interlayer coupling in magnetic multilayers.

For further information please contact:

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Electronic Structure Network in Argentina

Recently, we have received a very interesting letter from C. Osvaldo Rodriguez from La Plata in Argentina, who got to know about our Network through a collegue from Max-Planck-Institute in Stuttgart from whom he had received one of our Newsletters. It turnes out that last year a similar network to ours was set up in Argentina. Their network is of course much smaller than ours and consists of six nodes: *La Plata, Buenos Aires, Bariloche, Rosario, Santa Fe and Chaco*, involving in total a research community of 30 scientists interested in *Electronic Structure, First Principles Determination of Properties of Complex Systems*. It has some indirect financial support which allowed the scientists to meet 3 times last year, in the Comision of Energia Atomica (CNEA) Buenos Aires, to share know how, programs, etc., plus starting new collaborations. This year they held their meeting on 10th of March.

The Argentina's Network is very interested in our Network. They have asked to be placed on our mailing list and to have all our Newsletters to be sent to them via electronic mail. The e-mail address of their Network is: **electron@cnea.edu.ar**, and anything sent to this address gets distributed to all nodes and researchers involved. Our Argentinian collegues think that such an electronic link between our networks, whose interests overlap so much, will be very natural and beneficial to all.

At present, C. Osvaldo Rodriguez has also a link to EU through a contract with the group of Professor Niels Christensen in Aarhus to carry out research in the electronic structure field. Below we include some details on recently submitted papers that have resulted from their collaboration.

- M.G. Stachiotti, E.L. Peltzer y Blancá, R.L. Migoni, C.O. Rodriguez and N.E. Christensen,
  "*Lattice dynamics of the High T_c superconductor $HgBa_2CuO_4$*";
  accepted for publication in Physica C.

- I. Gorczyca, N.E. Christensen, E.L. Peltzer y Blancá and C.O. Rodriguez,
  "*Optical phonon modes in GaN and AlN*";
  accepted for publication in Phys. Rev. B.

- N.E. Christensen, J. Kudrnovsky and C.O. Rodriguez,
  "*Metamagnetic behavior in Fe_3Si and Fe_3Al*";
  to appear in Phys. Rev. B.

- M.G. Stachiotti, E.L. Peltzer y Blancá, R.L. Migoni, C.O. Rodriguez and N.E. Christensen,
  "*Theoretical determination of the lattice dynamics properties of the High T_c superconductor $HgBa_2CuO_4$*";
  accepted for publication in Journal for Superconductivity, Proceedings of the Miami Workshop on High Temperature Superconductivity, Miami Jan 1995, USA.

- C.O. Rodriguez, N.E. Christensen, Ruben Weht and Mariana Weissmann,
  "*Copper-oxygen derived bands close to the Fermi energy in $Bi_{2+x}Sr_{2-x}CuO_6$ (Bi2201)*";
  accepted for publication in Journal for Superconductivity, Proceedings of the Miami Workshop on High Temperature Superconductivity, Miami Jan 1995, USA.

- C.O. Rodriguez , Rubén Whet, Mariana Weissmann, N.E. Christensen and M.S. Methfessel,
  "*Surface effects on the electronic structure of Bi*2201";
  submited to Phys. Rev. Letters (Jan 95).

- N.E. Christensen, A.L. Ruoff and C.O. Rodriguez,
  "*Pressure strengthening-a way towards multimegabar pressures*";
  submitted to Phys. Rev. Letters (Feb 95).

- C.O. Rodriguez , Rubén Whet, Mariana Weissmann, N.E. Christensen and M.S. Methfessel,
  "*Are surface effects to be included in the study of the electronic structure of Bi*2201";
  to be published in Journal of Physics and Chemistry of Solids (Proceedings of the Stanford Conference on Spectroscopies in novel Superconductors, Stanford March 1995).

Full potential photoemission theory: Application to MgO and CaO

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Abstract

The full potential photoemission theory is applied for the first time to the alkaline-earths oxides MgO and CaO. This theory is a straightforward generalization of the one-step model of photoemission for the case of anisotropic, space-filling potentials and several atoms per unit cell. It allows the calculation of angle-resolved ultraviolet photoemission (ARUPS) and bremsstrahlung isochromat spectra (ARBIS) from compounds. The calculations are based on space-filling crystal potentials calculated self-consistently with the full potential Korringa-Kohn-Rostoker (KKR) band structure method. As a first application of this generalized one-step model we present calculated angle-resolved photoemission spectra from the (100)-surfaces of MgO and CaO and compare the results with corresponding experimental data. The results include the self-consistent band structures and a comparison of muffin-tin and full potential results. The overall agreement between experiment and theory is excellent.

(submitted to Surface Science)
Manuscript available from : mgrass@nostromo.physik.uni-osnabrueck.de

The Static, Dynamic and Electronic Properties of Liquid Gallium Studied by First-Principles Simulation

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Abstract

First-principles molecular dynamics simulations having a duration of 8 ps have been used to study the static, dynamic and electronic properties of ℓ-Ga at the temperatures 702 K and 982 K. The simulations use the density-functional pseudopotential method and the system is maintained on the Born-Oppenheimer surface by conjugate gradients relaxation. The static structure factor and radial distribution function of the simulated system agree very closely with experimental data, but the diffusion coefficient is noticeably lower than measured values. The long simulations allow us to calculate the dynamical structure factor $S(q,\omega)$. A sound-wave peak is clearly visible in $S(q,\omega)$ at small wavevectors, and we present results for the dispersion curve and hence the sound velocity, which is close to the experimental value. The electronic density of states is very close to the free-electron form. Values of the electrical conductivity calculated from Kubo-Greenwood formula are in satisfactory accord with measured data.

(submitted to Phys. Rev. B)
Revtex-file+postscript figures available from: j.m.holender@keele.ac.uk

The bulk and surface electronic structures of MgO

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Abstract

The bulk electronic structure of MgO is calculated from first principles including correlation effects within the *GW* approximation. The band gap, the position of the 2s O band, and the valence band width are in good agreement with experiment. From the quasiparticle bandstructure, optical transitions corresponding to the main optical absorption peaks are identified. The energy-loss spectra is also calculated and compared with experiment. The surface electronic structure of MgO(100) is calculated self-consistently within the local density approximation. It is found that states observed in a recent photoemission experiment outside the bulk allowed states are close to surface states.

(submitted to Phys. Rev. B, February 1995)
The REVTEX versions (without figures) or a hardcopy can be obtained from
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Generating tight-binding Hamiltonians with finite difference methods

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Abstract

A method is presented for deriving a nearest neighbor tight-binding Hamiltonian for electrons in solids, starting from a finite difference Hamiltonian with atomic spheres embedded in it. The space is divided into cells surrounding the atoms. The basis states of the tight-binding Hamiltonian are the eigenstates of the finite difference Hamiltonian in these cells with zero derivative boundary conditions at the cell boundaries. To calculate the matrix elements of the full Hamiltonian, the couplings over the links crossing the cell boundaries need to be restored which leads to a coupling between states in neighboring cells. The resulting tight-binding Hamiltonian is energy-independent. Typically about 100 states per cell are needed to achieve reasonable accuracy.

(submitted to Phys. Rev. B)
Revtex manuscript can be obtained from: jost@mentor.tvs.kun.nl

Magnetic Nanostructures: 4d and 5d Clusters on Ag (001)

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Abstract

We perform ab-initio calculations for the electronic structure of 4d and 5d transition-metal clusters at the (001) surface of Ag and determine the magnetic moments. Dimers, linear chains and plane islands are investigated, all showing a strong tendency for magnetism. We also compare our results with calculations for free clusters. Due to the hybridization with the substrate and with the adatoms in the clusters the maximum of the moment curve is shifted to large valencies. For all investigated structures Ru and Rh clusters are magnetic.

(submitted to Phys. Rev. Lett.)
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Use of Fermi Dirac Distribution in Ab-initio Green's Function Calculations

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Abstract

We present a practical method of introducing the Fermi Dirac distribution into ab-initio Green's function calculations. Based on a contour integration in the complex energy plane we evaluate the residua at a few Matsubara frequencies while the remaining integral is analysed by the Sommerfeld expansion. The total energy is calculated by the grand canonical potential for which a simple formula is given. We apply the method in calculations for the Ag(001) surface and for magnetic 4d adsorbate atoms on this surface.

(submitted to Phys. Rev. B)
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Electronic structure of crystalline and amorphous Nb_xMo_{1-x} alloys: Rigid versus rectangular bands

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Abstract

Ab-initio investigations of the electronic structure of disordered body-centred cubic and of amorphous Nb-Mo alloys are presented. We find that the crystalline Nb-Mo alloys are a rare example of an alloy system that conforms with the expectations of the rigid-band model. The electronic density of states of the amorphous Nb-Mo alloys differs drastically from that of the crystalline phases: it is rather close to the simple Friedel-model of a rectangular density of states. The origin of the striking differences in the band-structure and their consequences for the electronic properties, e.g. Collver-Hammond correlation in the superconducting transition temperatures, are discussed.

(submitted to J.Phys.:Condens.Matter)
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Uniaxial and planar magnetic anisotropy of thin transition-metal films

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Abstract

We present in novel approach to the calculation of magnetic anisotropies in crystals and in thin films. Our technique is based on selfconsistent real-space recursion calculations on a tight-binding-linear-muffin-tin-orbital (TB-LMTO)-Hubbard Hamiltonian including spin-orbit coupling and allowing for arbitrary orientations of the local spin-quantization axes. It allows to scan the magnetic energy continuously as a function of the orientation of the magnetic moment and thus to avoid the computational problems that plague other techniques. Applications are presented for bulk body-centred cubic iron and for face-centred cubic Fe monolayers on Cu(100) and Cu(111) substrates. We predict a perpendicular direction of the magnetic moment for Fe/Cu(100) and in-plane orientation of the spins for Fe/Cu(111), with anisotropiy energies of the order of 1 to 2 meV/atom. The technique is accurate enough for studying the weak in-plane anisotropies in Fe/Cu(111) that are of the order of 1 μeV/atom.

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Theoretical study of the Si(100) surface reconstruction

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Abstract

We present the results of a systematic study of the reconstruction of the Si(100) surface based upon total energies calculated within the framework of the local density approximation. We focus on the extent to which total energy *differences* may be calculated reliably by examining these differences for the ideal surface and four proposed reconstructions: $p(2 \times 1)$ symmetric, $p(2 \times 1)$ asymmetric, $p(2 \times 2)$ and $c(4 \times 2)$. The calculations were performed using norm-conserving pseudopotentials and a plane wave basis. The convergence of the total energy differences was assessed by varying the energy cutoff used to truncate the plane wave basis and the number of sampling points used to perform Brillouin zone (BZ) integrals over a large range. The effect of optimizing atomic geometries as a function of the energy cutoff and density of BZ sampling points was determined. With the exception of the $p(2 \times 2)$ and $c(4 \times 2)$ reconstructions whose energies only differ by 3 meV per dimer, we are able to unambiguously determine the energy ordering of the five systems studied. Disagreements between previous calculations can be largely understood in terms of the different energy cutoffs and BZ samplings used. The electronic structures of the different reconstructions are calculated and compared.

(to appear in Phys. Rev. B)

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Theory of the giant magneto-optical Kerr effect in $MnPt_3$ and PtMnSb

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Abstract

The magneto-optical (MO) Kerr effect in the manganese-platinum compounds $MnPt_3$ and PtMnSb is studied from first principles, using density-functional band-structure theory. The calculated Kerr spectra give a good description of the huge Kerr rotations found experimentally in these compounds. The origin of the Kerr rotation is discussed in relationship to the band structure and the spin-orbit (SO) interaction strength of Pt.

(Solid State Commun.**94**, 255 (1995))
Manuscript available from: peter@tmps08.mpg.tu-dresden.de

Low-temperature thermopower of Al-based dilute alloys

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Abstract

We report systematic calculations of the low-temperature diffusion themopower of Al-based dilute alloys with 3d and 4sp impurities, by solving self-consistently the linearized Boltzmann equation. The impurity scattering is described by the phase shifts obtained from self-consistent local-density-functional impurity-in-jellium calculations. Moreover, the influence of the full anisotropy of the Al Fermi surface on the scattering process is taken into account within the on-Fermi-sphere approximation. Our results explain successfully the experimentally measured variations of the thermoelectric power, except for Mn impurities. In this case, the presence of a narrow many-body resonance at the Fermi level in the localized-spin-fluctuations regime seems to be responsible for the large negative value of thermopower observed.

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Density functional theory without densities

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Abstract

Most of the basic ideas of the density functional theory (DFT) are shown to be unrelated to the fact that the particle density is used as the basic variable. After presenting the general formalism and a simple example unrelated to densities, we discuss various approaches to density functional theory on a lattice. One has proven useful for the understanding of various fundamental issues of the DFT. The exact Kohn-Sham band-gap and the band-gap in the local density approximation (LDA) are compared to the exact result for a one-dimensional model. As the interacting homogeneous system can be solved exactly no further approximation is needed to formulate the LDA.

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Analytical Molecular Orbitals and Band Structures of Solid C_{60}

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Abstract

Assuming icosahedral symmetry of the C_{60} molecule, we give analytical expressions for the h_u highest occupied and the t_{1u}^* and t_{1g} lowest unoccupied molecular orbitals (HOMO's and LUMO's). These are used for solid C_{60} to derive analytical one-electron Hamiltonians of minimal size, 5N×5N, 3N×3N, and 3N×3N, for respectively the h_u, t_{1u}^*, and t_{1g} subbands. Here, N is the number of C_{60} molecules per primitive cell. We use the nearest-molecule neighbor orthogonal tight-binding and single-MO approximations, both of which have been shown to work well for solid C_{60}. We explicitly consider structures with the C_{60} molecules at the sites of an fcc lattice: The uni, bi, and quadridirectional crystal structures with N=1, 2, and 4, respectively. The quadridirectional structure is that of pure and Na-doped C_{60} at low temperature. The bidirectional structure is usually considered a good approximation to the (unknown) structure of K and Rb-doped C_{60}. All nine subband Hamiltonians can be expressed in such a way that they have the same functional dependence of the Bloch vector. The number of inter-molecular transfer integrals is small, because we choose the MO's to transform in accordance with the common symmetry of the molecules. For each of the three structures and each of the three subbands, explicit expressions are given for the bandwidths and for the energies and wavefunctions at high-symmetry **k**-points. For the quadridirectional structure, this is done for a general angle of rotation φ.

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Electron states and luminescence transition in porous silicon

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Abstract

The theoretical analysis of two different wires of size 5x4 and 3x4, simulating porous Si has been performed through the Linear Muffin Tin Orbitals (LMTO) method in the Atomic Sphere approximation (ASA). All the core energies were selfconsistently computed and used to directly compare the energies of the quantum wires and that of the bulk Si, by aligning the 2p core level of a Si atom located at the center of the wire to that corresponding of bulk Si. The optical properties of the wires have been computed by evaluating the imaginary part of the dielectric function. The main results are: (i) the opening of the LDA gap is asymmetric: 1/3 of the widening is in the valence band, while 2/3 in the conduction band; (ii) the near band gap states originate from Si atoms located at the center of the wire; (iii) the imaginary part of the dielectric function shows a low energy side structure strongly anisotropic, that follows the blue shift of the gap and identified as responsible of the luminescence transition; (iv) the spatial localization of the valence and conduction band states involved in the luminescence transition shows that all the Si atoms of the wire are collectively involved.

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Ferromagnetism of 4d and 5d Transition Metal Monolayers on Ag(111)

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Abstract

We report systematic spin-polarized *ab initio* calculations for the electronic structure and magnetic moments of 4d (Mo, Tc, Ru, Rh, Pd) and 5d (Re, Os, Ir) transition metal overlayers on a Ag(111) surface. Allowing for ferromagnetic ordering nonvanishing magnetic moments were calculated for Ru ($1.23\mu_B$) and Rh ($0.67\mu_B$) among the 4d metals and for Ir ($0.05\mu_B$) among the 5d series. These results are compared to corresponding calculations for 4d and 5d overlayers on a Ag(100) surface and buried (100) interlayers in bulk Ag. On the basis of these results we discuss the dependence of magnetism of monolayers on substrate orientation and local atomic coordination.

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A Self-Consistent First-Principles Technique Having Linear Scaling

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Abstract

An algorithm for first-principles electronic structure calculations having a computational cost which scales linearly with the system size is presented. Our method exploits the real-space localization of the density matrix, and in this respect it is related to the technique of Li, Nunes and Vanderbilt. The density matrix is expressed in terms of localized *support* functions, and a matrix of variational parameters, $L_{\alpha\beta}$ having a finite spatial range. The total energy is minimized with respect to both the support functions and the $L_{\alpha\beta}$ parameters. The method is variational, and becomes exact as the ranges of the support functions and L matrix are increased. We have tested the method on crystalline silicon systems containing up to 216 atoms, and we discuss some of these results.

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Band theoretical investigation of the magneto-optical Kerr effect in Fe and Co multilayers

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Abstract

A band theory of the magneto-optical (MO) properties of solids, based on the first-principles spin-polarized, relativistic linear muffin-tin orbital method, is described. Two expressions of the relativistic electron-photon interaction matrix elements are implemented and their accuracies are investigated. It is found that the spin-polarized, relativistic band theory, together with the new expression of the photon absorption matrix elements, is able to give reliable optical conductivity and MO Kerr rotation spectra of bcc Fe which agree well with both experiments and recent calculations using a different method. The MO properties of several Fe and Co multilayers [$Fe(Co)_2$ Cu_6 fcc-(001), $FeCu(Ag)_5$ fcc-(001), bcc-Fe/fcc-Ag_5 (001), bcc-Fe_n/fcc-Au_5 (001) (n = 1, 3), Co_2Pd_4 fcc-(111) and Co_2Pt_m fcc-(111) (m = 1, 4, 7)] are then investigated theoretically. The calculated MO Kerr effect in all the mutlilayers except Co_2Pt_1 fcc-(111) is not larger than in bulk Fe and Co. Nevertheless, the results suggest that materials with larger Kerr rotations can perhaps be achieved by making Fe (Co) superlattices with ultrathin layers (few monolayers thick) of heavy elements possessing a partially filled d-band (e.g., Pt and Os). Kerr rotation spectra for Fe(Co)/Cu(Ag, Au, Pd, Pt) bilayers [i.e., a thin layer of Fe(Co) on the Cu(Ag, Au, Pd, Pt) substrate] are also obtained from the calculated optical conductivity tensors of Fe, Co, Cu, Ag, Au, Pd and Pt. It is found that the MO Kerr effect in the Fe(Co)/noble metal bilayers is considerably enhanced near the plasma edge of the substrate. This indicates that one can probably obtain good MO materials by fabricating Fe (Co) bilayers using nonmagnetic metals with a sharp plasma edge (e.g., Ag and Al) as substrates. Calculated Kerr rotation spectra of the Fe and Co multilayers as well as bilayers are in satisfactory agreement with available experiments. The spin and orbital magnetic moments as well as the Fermi contact and orbital hyperfine fields in the Fe and Co multilayers are also calculated. Possible correlations among the magnetic moments, hyperfine fields and MO properties of the Fe and Co multilayers are discussed.

(Phys. Rev. B 51, 1 May (1995) (in press))

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Giant magnetoresistance from first principles

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Abstract

The transport properties of Co/Cu multilayers are calculated from first principles in the ballistic regime. Magnetoresistances as large as 120% are obtained in the geometry with the current perpendicular to the interface plane. The *s*-*d* hybridization is found to play an essential role in giving rise to this giant magnetoresistance effect.

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Manuscript can be obtained from `schep@prl.philips.nl`

Phase diagram of the Cu-Pd surface alloy : a first-principles calculat ion

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Abstract

A method that combines electronic structure calculations with Monte Carlo simulations is applied to determine the phase diagram of the $CuPd$ surface alloy on a $Cu(001)$ substrate. The calculations are based on an effective Ising model with parameters as defined within the Generalized Perturbation Method and as calculated by means of the Linear-Muffin-Tin-Orbital method. The formation of the ordered $c(2 \times 2)$ phase of the $CuPd$ surface alloy on the $Cu(001)$ substrate is discussed. The order/disorder temperature of the $c(2 \times 2)$ phase as well as the phase diagram is calculated using pair interactions corresponding to the 50:50 composition as well as concentration dependent pair interactions.

(submitted to Phys. Rev. B)
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Magnetism of 4d and 5d adlayers on Ag(001) and Au(001): comparison between a non–relativistic and a fully relativistic approach

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Abstract

The magnetic properties of mono– and double layers of Ru, Rh, Pd, Os, Ir and Pt on Ag(001) and Au(001) are investigated using the scalar–relativistic and the fully relativistic spin–polarized Screened KKR method. It is shown that, in particular, for the case of the Ir monolayers and Pt double layers a non–relativistic approach is no longer valid, since a magnetic ground state would be predicted, while a relativistic description yields a non–magnetic ground state.

(Phys.Rev.B, in press (1995))
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Interlayer magnetic coupling: effect of interface roughness

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Abstract

The effect of structural interface imperfections on the interlayer magnetic coupling is studied theoretically by considering: (i) a macroscopic model of roughness for possible fluctuations of spacer thickness, and (ii) a microscopic model of interdiffusion at ideal interfaces. For the Co/Cu/Co(001) system, we found a dramatic decrease of the amplitudes of the oscillations even for a small amount of interface imperfections. The influence of roughness is particularly strong for the short period oscillations. Our results clearly confirm the decisive role of interface scattering for the strength of the exchange coupling and indicate a possible source of discrepancy between ab-initio calculations and experiment.

(submitted to Phys. Rev. B)
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Magnetic Anisotropy of Iron Multilayers on Au(001): First Principles Calculations in Terms of the Fully Relativistic Spin–Polarized Screened KKR Method

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Abstract

In order to treat the orientation of the magnetic field at surfaces properly, the spin–polarized fully relativistic version of the Screened Korringa–Kohn–Rostoker method for semi-infinite systems is presented. Magnetic anisotropy energies up to six iron layers on Au(001) are calculated by using the 'force theorem', predicting a change from a perpendicular to a parallel magnetization for a layer thickness between 3 and 4 layers of Fe, in very good agreement to experimental observations. In particular, the magnetic anisotropy energy is discussed in relation to the orbital magnetic moment and to the orientation of the magnetic field when changed continuously.

(Phys.Rev.B, in press (1995))
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THE INFLUENCE OF SHORT RANGE ORDER ON THE ENERGETICS OF Ni-RICH NiAl ALLOYS[1]

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Abstract

Total energy calculations for Ni-rich β-phase NiAl have been performed using the large system multiple scattering (LSMS) method. The large samples used to model the alloys involved up to 128 atoms per cell, and were constructed to have the experimental short range order (SRO) parameters. Both short range ordering and charge transfer effects are automatically taken into account in the calculation. The calculated formation energies of both stoichiometric and non-stoichiometric compounds are in excellent agreement with experiment.

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Correlation energy functionals for *ab initio* calculations. Application to transition metals.

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Abstract

The method for including strong correlation effects in self-consistent electronic structure calculations in solids is presented. On the basis of mean-field type (Gutzwiller-type) approximation the correlation energy functional is obtained which depends on the partial electron density. In turn, the variation of this functional yields the non-local effective potential. Two possible variational procedures are tested: variation of the functional over occupation numbers only and over both occupation numbers and LMTO-ASA wave function. The LMTO-ASA calculations for a number of 3d and 4d transition metals are carried out. The results are compared with those for density functional calculations. Quantitative estimates of correlation renormfactor for the band width "dynamical" narrowing in these metals are presented.

(submitted to Phys. Rev. B)

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First-principles theory of spontaneous magnetoresistance anisotropy and anomalous Hall effect in disordered ferromagnetic alloys

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Abstract

A fully relativistic first-principles theory of the conductivity of disordered magnetic alloys based on the Kubo-Greenwood formalism and the spin-polarised relativistic Korringa-Kohn-Rostoker coherent-potential approximation (SPRKKR–CPA) method is presented. This new approach allows for a treatment of spin-orbit-coupling and spin-polarisation on an equal footing and to account properly for the reduction in symmetry caused by the simultanous presence of them that way. Consequently – in contrast to previous approaches – one has access to a parameter-free theoretical description of the spontaneous magnetoresistance anisotropy and the anomalous Hall resistivity of magnetic alloys. A first application to the system Fe–Ni yields results which are in very satisfying agreement with experiment.

(submitted to Phys. Rev. Lett.)
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Periodic Planar Jellium Approximation to Implanted Metal Surfaces

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Abstract

The periodic planar jellium (PPJ) approximation to the metal surface has been introduced some time ago in an attempt to incorporate the surface anisotropy into the solution of the metal surface. The PPJ approximation is the natural zeroth order approximation of a solution to the semi-infinite metal that is based on expanding wave functions and potentials in a coordinate dependent Fourier series in terms of 2D plane waves. In the PPJ approximation the ionic charge takes the form of uniform planar charge distributions in planes parallel to the surface or the interface. Recently, the PPJ model attracted new interest in the description of metallic and/or magnetic overlayers. We are currently interested in using the PPJ model for describing metallic overlayers and implanted metal surfaces with alkali metal atoms. In this work, preliminary results from applications on adsorbed and implanted surfaces are presented.It is shown that the implanted metal surface exhibits specific characteristics that result from the changes in the electrostatic surface dipole moment which in turns depends strongly on surface relaxation.However,the experimental lowering of the work function upon implantation cannot be accounted for by these factors only and other mechanisms that can be modeled by a concentration dependent ionic valency, should be taken into account.

(accepted by Computational Materials Science)
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An algebraic representation of the linear-analytic tetrahedron method

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Abstract

We present a new formulation of the tetrahedron method for calculating Lindhard sums in susceptibility calculations. Using an analytic approach rather than the usual geometric interpretation, we provide a general algebraic form for the integral. Our result is much more compact and less complicated than the geometric approach and involves the minimum of calculation. The ordering and subdivision of tetrahedra in the geometric approach is obviated. Our analytic approach may be readily applied to other microcell geometries and is demonstrated in this paper for both the tetrahedron microcell as well as the geometrically complex parallelepiped microcell.

(to appear in Comp. Phys. Comm.)
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Magnetovolume effect of RMn_2 Laves phase compounds

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Abstract

We calculate self consistently the band structure of the antiferromagnetic C15 Laves phase compounds YMn_2 and $TbMn_2$ using the first principles LMTO-ASA method. By studying the variation of the total energies with respect to lattice spacing for various magnetic states we can account for the large magnetovolume effect which occurs in these compounds upon transition to the antiferromagnetic state. Our self consistent calculations on YMn_2 show that Y is paramagnetic whereas for $TbMn_2$ we find a ferromagnetic moment for the Tb atom. We also find that the changes in the staggered moment are relatively smaller for the $4s$- and $4p$-orbitals than for the $3d$- orbital which contributes most of the moment. We give the projected density of states for each spin on each of the atoms and analyze and discuss their variation with the lattice spacing.

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Susceptibilities using first principles band structures II

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Abstract

We have completed a program for the parallel calculation of the fully interacting static susceptibility from first principles LMTO band structures using methods and programs developed in previous papers. We present the results for the many-body enhanced static magnetic susceptibility $\chi(\mathbf{q})$ for Pd and fcc γ-Mn and discuss how the simple Stoner criterion and its extension can give an incorrect physical picture of magnetic instabilities. We discuss the important local field effects which necessarily arise from an *ab initio* calculation of χ and give a more detailed discussion of the antiferromagnetic instabilities in fcc γ-Mn.

(to appear in Physica B)
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Ab Initio calculation of spin-waves in Iron and Nickel

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Abstract

Ab initio LMTO calculations have been performed to obtain the dynamic many-body enhanced magnetic susceptibility for both Nickel and Fe. The dispersion relationship of the collective excitations obtained are in excellent agreement with experiment. Spin waves are found to persist out to the Brillouin zone edge although damped by the Stoner excitations. Although we find both optic and acoustic branches for the spin waves in Fe we do not find the optic branch for Ni. This is in contrast to the calculation of Trohidou et al who used a parametrised interaction.

(to be submitted to Phys. Rev. Lett.)
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HIGHLIGHT OF THE MONTH

Comment on:

Porous Silicon

by O.Bisi

University of Trento, Italy

1 Introduction

The rise of the communication high-way, the increased speed of computers, the diffusion of multimedia systems and the use of intelligent control systems are a few examples where a need for photonic applications has emerged. In this field the III-V and II-VI semiconductor compounds have been the materials to develop photonic applications up to now. Silicon has not been considered until the early nineties when Canham demonstrated that a Si based material was able to emit visible light at room temperature with quantum efficiencies approaching 10% [1, 2]. This material is porous Si (p-Si) which is obtained by electrochemical dissolution of Si. Following this discovery a large effort has been renewed to develop alternative Si based materials where visible light emission is predictable and observable. The driving idea is to realise a material where confinement, passivation and short-range crystallinity are all present. Indeed all these three items play a crucial role in p-Si.

2 How To Form Porous Silicon

Porous Si is obtained through electrochemical dissolution of Si in a solution of fluoridric acid and water or ethanol. This electrochemical process was initially developed for electro-polishing of Si wafers. When the current is low enough no electro-polishing occurs and a regime is entered where a random network of micropaths entering the Si is formed. This regime is that characteristic to form p-Si. As a result, a sponge-like layer is formed in the Si

wafer composed by porous and crystalline parts. The p-Si skeleton is composed by a hank of Si wires. Both n-type or p-type doped Si can be used. As holes are necessary to dissolve Si, one has to illuminate the wafer for etching n-type Si.

The thickness of the porous Si layer is usually around 1-10μm. The porosity, P, is measured through a gravimetric technique where the weight (m1) of the sample before the attack, the weight (m2) after the attack, and the weight (m3) after dissolution of the porous layer in KOH are recorded, then P=(m1-m2)/(m1-m3). The p-Si layers so formed have porosities dependent on the electrochemical parameters. The effect of the different parameters on the resulting layer is as follows [3]: increasing the current increases the porosity, increasing the etching time increases the p-Si layer thickness, increasing the HF concentration decreases the porosity, increasing the doping density of the sample decreases the porosity. Some formation mechanisms for p-Si have been proposed. These are reviewed in Refs. [4, 5, 6, 7, 8, 9].

It is worth-noticing that the porous Si samples freshly etched are different from the aged ones. In fact the p-Si samples are subjected to an aging process in which the chemical characteristics of the nano-crystal surface and of the surrounding matrix change. The nano-crystal surface is rich in hydrides for freshly etched samples while it is covered by an oxide matrix in aged samples. This is evidenced in the Auger lineshape of the LVV Si transition [10]. The Si lineshape changes from one characteristic of a covalent bonded Si atoms to one of an ionic bonded Si atom, i.e. H has been replaced by O. Theoretical calculations of the Si LVV lineshapes show that in the region of freshly etched samples investigated by the Auger probe the Si-H_2 bond is predominat [11]. The aging process induces a peculiar blue-shift of the visible luminescence band because the thin oxide layer formed on the surface of the Si nano-crystals reduces the size of the inner crystalline part. Sometimes an increase in the luminescence intensity is also measured in aged samples.

3 The Quantum Confinement Model

Room temperature visible photoluminescence is seen with the naked eyes in p-Si. The colour can be varied over the whole visible spectrum (from red, 1.8 eV, to green, 2.4 eV) by appropriate treatments which could involve oxidation steps. The spectral position of the luminescence band depends on the porosity, and shows a blue shift with increasing porosity. This observation together with TEM imaging [12] led Canham to propose the quantum model to explain the visible luminescence band of p-Si. In this model, p-Si is formed by a disordered array of undulating quantum wires (1-dimensional systems). Further refinements of the model consider the presence of interconnected quantum-dots (QD, 0-dimensional systems) where the excitons are confined.

According to the simple particle-in-a-box example [13], the electron-hole transition energy

is larger than the Si energy gap because it results from the sum of the Si energy gap, the electron and the hole confinement energies minus the exciton binding energy. In fact the excitonic recombination in p-Si occurs in the visible, while the Si energy gap is 1.1 eV. Since high porosity samples have more voids with respect to low porosity samples, one expects smaller Si nano-crystal sizes for the high porosity samples, i.e. a large quantum confinement, and, consequently, a blue shift in the luminescence. Indeed this is observed, which strongly supports the quantum confinement model. The 0.3 eV width of the visible band is explained by the distribution in the nano-crystal size, to which corresponds an energy distribution of the excitonic recombination energies.

Another direct evidence of the presence of nano-crystalline Si comes from Raman measurements [14]. A characteristic softening and broadening of the Si crystalline optical phonon mode is observed and associated with the confinement of the optical phonon in the nano-crystals. In addition, a contribution of an amorphous layer is present. The relative intensity of the two structures is sample and excitation wavelength dependent. By the TEM images and these data, a model of p-Si emerges where voids and nanocrystals interconnected by an amorphous matrix form the porous layer.

A further evidence of the validity of the model is provided by excitation spectroscopy [15]. In these experiments the luminescence is excited by changing the excitation energy. When the exciting energy is sufficiently low an emission band is measured with a stepped increase on the high energy side. The steps are attributed to phonon-assisted recombinations of the excitons. The energy separation of the steps is that typical of crystalline Si phonons. Hence the visible band is due to excitonic emission which are quantum confined (see the spectral position of the emission band) in crystalline Si (note the phonon energies). This result rules out other possible models for the emission either based on surface states or on chemical species.

From a theoretical point of view studies of H-terminated Si quantum wires based on both semiempirical [16, 17, 18, 19] and first principles local density calculations [20, 21, 22, 23] pointed out that Si atoms form a direct gap material, if arranged in a quantum wire geometry. The calculation of the ϵ_2 function has been used to investigate the origin of the luminescence transition. Buda et al. [22] found a low energy structure of the component of ϵ_2 along the direction parallel to the axis of the wire, characteristic of the quantum wire structure and strongly dependent on the size of the wire. This dependence can explain the blue shift of the luminescence band, found on varying the porosity of p-Si. Therefore these authors suggest that this structure is responsible for the luminescence transition. The origin of this luminescence band is still under debate: according to a cluster calculation it originates from quantum confinement effect [24], while other authors point out the importance of surface states [25], or the presence of a Si cristalline inside the wire [20, 26]. We have recently shown

that all the Si atoms of the wire are collectively involved in the luminescence transition [27].

4 The Siloxene model

Stutzmann and co-workers proposed Siloxene (a particular Si:O:H compound whose chemical formula is $Si_6O_3H_6$) as the luminescent agent in p-Si [28]. Very recently, Brandt and Stutzmann [29] complemented the Siloxene model by assuming that a unique unit cell exists in several Si based systems which exhibits luminescence. This unique cell is composed by a six Si atom ring and is proposed to act as the radiative centre in p-Si, a-Si:H, siloxene compounds, substoichiometric alloys of Si. The Siloxene model seems not suitable to interpret all the experimental data. Among them, the strong luminescence in p-Si samples grown in the absence of oxygen and the EXAFS analysis of freshly etched p-Si, showing a clear difference between the Si neighbors in Siloxene and in porous Si [30]. It may be that a Siloxene-like compound exists in the surface layer of the oxidized p-Si samples, even if its presence is not necessary in order to obtain luminescence from Si.

5 Perspectives

Many questions on p-Si are open and first-principles calculations and new ideas are necessary to investigate this field. For example a full description of the optical properties of a Si wire (ϵ_1, loss function, etc.) is still lacking. Furthermore the system studied up to now consists of an H-passivated quantum wire, ideal quantum wire with crystalline lattice and the simplest passivating agent, hydrogen. More realistic models should include the effect of disorder, both in the surface of the wire, by considering the formation of a disordered layer of unknown composition, and in the topology of the structure. It is important to understand why the replacement of hydrogen by oxygen does conserve luminescence. At present this point is not fully understood and calculations for O-passivated quantum wires are lacking. In addition all the first-principles calculations on Si quantum wires do not include exchange-correlation effects beyond LDA. To my knowledge the only evaluation consists of an average between bulk and molecular self-energies [23].

A second point regards other forms of luminescent silicon. It is now generally accepted idea that p-Si opened the way to a new class of nanostructures based on Si [31]. The driving idea is to obtain a material where confinement, passivation and short-range crystallinity are all present. It is not clear what system will be the best for photonic applications.

At last, a few words on electroluminescence, i.e. the emission of light after excitation with carrier injection. Light emitting diodes (LED) have been fabricated which operate at room

temperature though with a very low efficiency [10]. Many problems have to be solved in order to obtain efficient LED based on p-Si. The interested reader is referred to the paper of Lang et al. [32]. Maybe p-Si will not result as the right material but it has had the great merit to indicate the essential ingredients for obtaining a good light emitter based on Si.

References

[1] L. T. Canham, Appl. Phys. Lett. **57**, 1046 (1990).

[2] L.T. Canham, in *Optical Properties of Low Dimensional Silicon Structures*, edited by D. Bensahel, L.T. Canham, and S. Ossicini, Kluwer, Dordrecht (1993), p. 81.

[3] M. I. J. Beale, J. D. Benjamin, M. J. Uren, N. G. Chew, and A. G. Cullis, J. Crystal Growth **73**, 622 (1985).

[4] H. Foll, Appl. Phys. A **53**, 8 (1991).

[5] R. L. Smith and S. D. Collins, J. Appl. Phys. **71**, R1 (1992).

[6] *Porous Silicon*, edited by Zhe Chuan Feng and R. Tsu (World Scientific Publishing Co., New York 1995)

[7] *Porous Silicon Science and Technology*, edited by J.-C. Vial and J. Derrien (Les Editions de Physique, Paris 1995).

[8] special issue Thin Solid Films vol. 255 (1995).

[9] *Microcrystalline and nanocrystalline semiconductors*, edited by L. Brus, R. W. Collins, M. Hirose and F. Koch, MRS Symposia Proceedings No. 358 (Materials Research Society, Pittsburgh, 1995).

[10] L. Pavesi, M. Ceschini, G. Mariotto, E. Zanghellini, O. Bisi, M. Anderle, L. Calliari, M. Fedrizzi, L. Fedrizzi, J. Appl. Phys. **75**, 1118 (1994).

[11] L. Dorigoni, L. Pavesi, O. Bisi, L. Calliari, M. Anderle, S.Ossicini and F.Bernardini, submitted to the EMRS spring meeting (Strasbourg, May 22-26, 1995), and to be published.

[12] A. G. Cullis and L. T. Canham, Nature **353**, 335 (1991).

[13] S. S. Iyer and Y.-H.Xie, Science **260**, 40 (1993).

[14] J. M. Perez, J. Villabo, P. McNeill, J. Prasad, R. Cheek, J. Kelber, J. P. Estrera, P. D. Stevens, and R. Glosser, Appl. Phys. Lett. **61**, 563 (1992).

[15] P. D. J. Calcott, K. J. Nash, L. T. Canham, M. J. Kane, and D. Brumhead, J. Phys: Condens. Matter **5**, L91 (1993).

[16] G. D. Sanders and Y. -C. Chang, Phys. Rev.B **45**, 9202 (1992).

[17] C. Delerue, G. Allan, and M. Lannoo, Phys. Rev. B **48**, 11024 (1993).

[18] C-Y. Yeh,S. B. Zhang and A. Zunger, Appl. Phys. Lett. **63**, 3455 (1993).

[19] H. M. Polatoglou, Journ. of Lumin. **57**, 117 (1993).

[20] A. J. Read, R. J. Needs, K. J. Nash, L. T. Canham, P. D. J. Calcott, and A. Qteish, Phys. Rev. Lett. **69**, 1232 (1992).

[21] T. Ohno, K. Shiraishi, and T. Ogawa, Phys. Rev. Lett. **69**, 2400 (1992).

[22] F. Buda, J. Kohanoff, and M. Parrinello, Phys. Rev. Lett. **69**, 1272 (1992).

[23] M. S. Hybertsen, and M. Needels, Phys. Rev. B **48**, 4608 (1993).

[24] Fu Huaxiang, Ye Ling and Xie Xide, Phys. Rev. B **48**, 10978 (1993).

[25] F. Koch and V. Petrova-Koch, in Ref.[6], pag. 133.

[26] Y. H. Xie, M. S. Hybertsen, W. L. Wilson, S. A. Ipri, G. E. Carver, W. L. Brown, E. Dons, B. E. Weir, A. R. Kortan, G. P. Watson, and A. J. Liddle, Phys. Rev. B **49**, 5386 (1994).

[27] L. Dorigoni, O. Bisi, F.Bernardini and S.Ossicini, submitted to the EMRS spring meeting (Strasbourg, May 22-26, 1995), and to be published.

[28] M. S. Brandt, H. D. Fuchs, M. Stutzmann, J. Weber and M. Cardona, Solid State Commun. **81**, 307 (1992).

[29] M. S. Brandt and M. Stutzmann, Solid State Commun. **93**, 473 (1995).

[30] S. L. Friedman, M. A. Marcus, D. L. Adler, Y. -H. Xie, T. D. Harris, and P. H. Citrin, Appl. Phys. Lett. **62**, 1934 (1993).

[31] O. Dag, A. Keperman and G. A. Ozin, Advanced Materials **7**, 72 (1995).

[32] W. Lang, P. Steiner and F. Kozlowski, Journal of Luminescence **57**, 341 (1993).