HCM Newsletter

Ψ_k Network

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

Number 7 February 1995

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Editorial

First of all we would like to welcome you to the first Newsletter of this calendar year. As in the past year, we would like to invite you to submit to our future Newsletters abstracts of your recently submitted papers and any other information, including comments on scientific papers or small review papers for our **Highlight of the Month section**, etc. Moreover, we would like to encourage you to acknowledge the Network in your publications resulting from genuine collaborations within the Network, and to send us all the details of such publications.

In this Newsletter, as usually, the abstracts are placed at the end of the Newsletter, just before the section **Highlight of the Month**. In the latter you can find an article by *Hubert Ebert, G.-Y. Guo and J. Banhart* on "*Galvano-magnetic and Magneto-optical Properties of Transition Metal Systems*".
In the section **News from the Network** we have given some preliminary information on the big conference of the Network, to be held on 18-21 September 1996 in Schwäbisch Gmund (Germany), as discussed at the last *Network's Management Board Meeting* on November 4, 1994. In this section we have also summarised the **Annual Progress Report** of the Network's activity that was submitted to Brussels at the end of December 1994.
In the section **News from the Working Groups** you can find reports on collaborative visits and/or workshops. Moreover, there you can find 2^{nd} **circular of the workshop** on *Spin-Orbit Influenced Spectroscopies of Magnetic Solids*, and the **first announcement of the hands-on workshop** on *Full-Potential LAPW calculations with the WIEN95 code*, as well as an announcement of a **Study Weekend at Daresbury Laboratory (UK)**, all in April.
Also, enclosed are **announcements** of a position available at the University of Cagliari, a post-doc fellowship at the Aristotle University of Thessaloniki (Greece), and post-doc positions at the University of Cambridge (UK).

We have a disappointing message for those non-funded members from Central and Eastern European Countries for whom we were seeking funds from Brussels. Our supplementary proposal PECO94 for Cooperation in Science and Technology with Central and Eastern European Countries and with the New Independent States of the former Soviet Union has failed to get funded by Brussels. At the moment there is no possibility to reapply. However, there may be other opportunities in future.

Could the non-funded nodes, however only from the European Union countries, please send us a.s.a.p. their **detailed affiliations**, including e-mail address, telephone and fax numbers, and inform us how many people belong to a particular node. This information is necessary for the enlargement of the Network within the presently available funds. We expect to extend the funding to about thirty, yet non-funded, nodes.

Please note that the *anonymous ftp directory* containing all the newsletters has changed name from **HCM.newsletters** to **psik-network**.
So, the procedure of anonymous ftp is as follows:
(1) ftp ftp.dl.ac.uk
(2) login as *anonymous* and give *your e-mail address* as the password
(3) cd psik-network

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**

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News from the Network

1 Network's Conference

Place and Time:

At the last *Network's Management Board* meeting it was agreed that the Network's Conference is going to take place on 18-21 September 1996 in Schwäbisch Gmund (about 45 km from Stuttgart airport).

It was suggested to introduce the date of the conference to the Karlsruhe Information Center, Physics Today, MRS, and Europhysics News to prevent other conferences to be arranged at the same time slot. The title of the conference is going to be: ψ_k-**Conference**, organised by the **HCM-Network** on "*Ab-initio (from electronic structure) calculation of complex processes in materials*".

Participation and Financial Support:

About 300 participants are expected. The Network should pay for the invited speakers maximum 1000 ECU, but there should also be funding for the members of the Network, especially the young researchers, PhD students etc., at about 300 ECU per person. Detailed funding policy with respect to the latter still needs to be worked out. Funding needs to be flexible and only for those who really need it. Nobody should be excluded but preference should be given to young people. The Network should estimate how many participants and at which value can be subsidised. Moreover, the Network should seek additional funds for subsidising participants from Central and Eastern European countries; eg. International European Conference Fundation. There should be **a conference fee of about 80 ECU**.

Abstracts and Proceedings:

The deadline for the abstracts should be very strict. The abstracts should be extended, i. e. maximum one page. All the abstracts will be available by e-mail and/or from World Wide Web before the conference. All abstracts will be accepted (no refereeing), but only poster-presentation will be guaranteed.

It was suggested to encourage as many posters as possible.

It was decided that there would be no conference proceedings.

Main Topics of the Conference:

- Density Functional Molecular Dynamics Simulation: techniques 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 (Parallelization)
- Applications to All Aspects of Condensed Matter and Materials Science including:
  Reactions at Surfaces
  Magnetic Multilayers
  Theories of Spectroscopies
  Molecular Materials
  Carbon Structures
  Semiconductor Heterostructures and Quantum Wires
  Oxides/Metal Interfaces

Conference Structure:
Three parallel symposia are planned. Moreover, one could think of the Beer Postersession subsidised by a foreign company. Also, manufacturers and publishers could be invited.

2 Progress Report, 1 January 1994-15 December 1994

HCM ψ_k-Network on Ab initio (from electronic structure) calculation of complex processes in materials

Contract Number: CHRXCT930369

Preamble

This network is characterized by the large number of nodes (40) and more than 200 participating researchers. The network aims to promote excellence in the subject of quantum mechanical calculations for electronic properties of solids through collaborations accross Europe including helping those in smaller or new or isolated research groups.

To operate efficiently as such a large network we have established a broadcast e-mail service and we publish a bimonthly newsletter which is e-mailed to more than 200 researchers with network information on workshops, collaborations and scientific highlights. We run an abstract service through this newsletter and also through anonymous ftp and World Wide Web. Our success can be measured by the fact that we are submitting in January 1995 a request to expand this Network to more than 70 nodes.

Nine workshops have been organised sofar. Two of them were courses where use of the latest electronic structure codes for solids were taught. Two of them were on techniques for electronic structure studies, namely Greens functions and parallel algorithms. Five workshops were devoted to leading edge projects in magnetism, superconductivity, improved density functionals, large systems and electrons in different dimensions.

Twenty collaborative visits have taken place, ranging from joint development of computer codes, initiating of collaborative projects to continuation of mature collaboration. This has resulted in six publications sofar. To mention but a few of our highlights, I am selecting the following:

- A collaboration between Fritz-Haber-Institut (Berlin, Germany), and (Tech. Univ., Vienna, Austria) in the development of a code for direct evaluation of atomic forces into the LAPW code.
- A collaboration between MPI Stuttgart (Germany), Daresbury Laboratory (UK), and University of Bristol (UK) to solve the BdG equations for $YBa_2Cu_3O_7$.
- A collaboration between MPI Stuttgart (Germany) and Cavendish Laboratory (Cambridge, UK) on order (N) methods.
- A collaboration between the group of John Inglesfield (Nijmegen) and Charles Patterson (Dublin) on dielectric response functions.
- A collaboration between France/ Germany/ Switzerland involving C. Koenig, M. Springborg and P. Blöchl on Complex Molecular Materials.
- A collaboration between J.L. Martins (Portugal) and Van Camp and Van Doren (Belgium) on the phase transformations in $AlAs$ and further collaboration on nitride materials.
- A collaboration between Stefanou (Univ. Athens, Greece) and the group in Jülich (Germany) on the electronic and magnetic impurities in solids.

As it happens, this year the stress was put on the training aspects and a variety of meetings, to feed the scientists participating in the Network with a wide input for collaborations. Therefore, instead of six planned workshops, there have been nine workshops or meetings, and only 50% of the planned collaborative visits have taken place. The Network is extremely large and developes in a very dynamical way. Many collaborations have already started as a result of all the meetings and there are many more to come. Moreover, the Network has decided to invite a number of scientists from outside the Network to participate in many of the workshops and meetings as experts/consultants in a given scientific topic or additional scientists (marked as ADSC below). This has turned out to be extremely beneficial to the whole Network and is resulting in an expansion of the Network to more than 70 teams (from EU countries). Below we enumerate the names of the experts/consultants and additional scientists.

Factual Information

Sofar, this Network has funded 3 Network Management Board Meetings: *1st Network Management Board's Meeting, MPI Stuttgart (Germany) , 24th September, 1993.*

2nd Network Management Board's Meeting, University of Paris, 4th March, 1994.
3rd Network Management Board's Meeting, University of Paris, 4th November, 1994.

9 workshops:

- *Green functions and CPA:* Muenster 25 March 1994
- *Dynamical Order N Tight Binding (DONTB):* Stuttgart 11-12 April 1994
- *Magnetic Surfaces, Interfaces and Multilayers:* Vienna 29-31 May 1994
- *Ab-initio Molecular-Dynamics Calculations of Structural, Elastic, and Vibrational Properties of Polyatomic Systems:* Berlin 3-7 October 1994
- *Hands-on the TB-LMTO-ASA computer program:* Stuttgart 24-28 October 1994
- *The Aarhus Workshop on Quantum Theory of Solids: Improved Density Functionals:* Aarhus 9-10 June 1994
- *Solving the Bogoliubov-de Gennes Equations for Superconductors:* Bristol 29-30 October 1994
- *Electrons in Different Dimensions:* Varenna 8-14 May 1994
- *Parallel Algorithms for Large Systems:* Taormina 26-28 November 1994

20 collaborative visits (secondements):

- **M. W. Finnis** (from *MPI für Metalforschung, Stuttgart* to *Cavendish Laboratory Cambridge*), 30th October-4th November, 1994.
- **V. Heine** (from *Cavendish Laboratory, Cambridge* to *Technical University, Copenhagen-Lyngby*), 6-9th January, 1994.
- **J.L. Martins** (from *INESC Lisbon* to *University of Antwerp*), 19-23rd January, 1994.
- **C. Patterson** (from *Trinity College,Dublin* to *Catholic University, Nijmegen*), 24-25th January, 1994.
- **Z. Szotek** (from *MPI für Festkorperforschung, Stuttgart* to *University of Paris*), 2-6th March, 1994.
- **W.M. Temmerman** (from *MPI für Festkorperforschung, Stuttgart* to *University of Paris*), 2-6th March, 1994.
- **G.Y. Guo** (from *Daresbury Laboratory* to *IFF,KFA-Jülich*), 25-26th April, 1994.
- **S. Blügel** (from *IFF,KFA-Jülich* to *Technical University of Vienna*), 23rd May-20th June, 1994.
- **B. Ginatempo** (from *University of Messina* to *University of Warwick*), 9-20th July, 1994.

- **M. W. Finnis** (from *MPI für Metalforschung, Stuttgart* to *Cavendish Laboratory Cambridge/Keele University*), 1-31st August, 1994.
- **V. Heine** (from *Cavendish Laboratory, Cambridge* to *ERC Conference, Gausdal, Norway*), 27 August-1st September, 1994. The purpose was to speak to the Conference participants on behalf of the Network.
- **B. Kohler** (from *Fritz-Haber-Institut Berlin* to *Technical University, Vienna*), 5-9th September, 1994.
- **V. Heine** (from *Cavendish Laboratory, Cambridge* to *Fritz-Haber-Institut, Berlin*), 2-5th October, 1994.
- **G. Bihlmayer** (from *University of Vienna* to *University of Cagliari*), 21-26th October, 1994.
- **R. Podloucky** (from *University of Vienna* to *University of Cagliari*), 21-26th October, 1994.
- **C. Demangeat** (from *IPCMS Strasbourg* to *IFF,KFA-Jülich*), 2-5th November, 1994.
- **A. Burkhardt** (from *MPI für Festkorperforschung, Stuttgart* to *Daresbury Laboratory*), 13-15 November, 1994.
- **S. Simak** (from *University of Rennes* to *University of Konstanz*), 26th November-11th December, 1994.
- **C. Patterson** (from *Trinity College,Dublin* to *Catholic University, Nijmegen*), 15-17th December, 1994.
- **Dietmar Herrendorfer** (from *Trinity College,Dublin* to *Catholic University, Nijmegen*), 15-17th December, 1994.

and **42 visits** of visiting scientists/consultants (from outside the Network) to various workshops. Moreover, the Network funds a half of the salary of the scientific secretary: Dr. Z. Szotek (Belgian nationality and based in Daresbury Laboratory, UK).

Joint Publications

Sofar only the following publications have been finalised, although there are more in the pipeline.

- C.F. Hague, J-M. Mariot, G.Y. Guo, K. Hricovini, and G. Krill, "Coster-Kronig contributions to magnetic circular dichroism in the $L_{2,3}$ x-ray fluorescence of iron", (to be published in Phys. Rev. B (rapid communication).
- S. Crampin, M. Nekovee and J.E. Inglesfield, "The embedding method for confined quantum systems", (submitted to Phys. Rev. B).
- S. Crampin, M.H. Boon and J.E. Inglesfield, "Two- and three-dimensional aspects of surface state confinement", (to be published in the Proceedings of the "Electronic surface and interfaces states on metallic systems" meeting, Bad Honnef, 17-20 October 1994 (World Scientific)).

- P.E. Van Camp, V.E. Van Doren, and J.L. Martins, "Structural Phase Transformation of Aluminum Arsenide", (to be published in the Proceedings of the International Conference on 'The Physics of Semiconductors', Vancouver (Canada), August 10-14, 1994).
- M.W. Finnis, R. Kaschner, C. Krause, and J. Furthmm̈ller, and M. Scheffler, "The interaction of a point charge with a metal surface: theory and calculations for (111), (100) and (110) aluminum surfaces", (submitted to Journal of Physics: Condensed Matter).
- N. Papanikolaou, N. Stefanou, R. Zeller, and P. Dederichs, "Magnetic Behaviour of Transition-Metal Impurities in Alkali-Earth Metals", (submitted to Phys. Rev. B).

Cost Statement 24 September 1993 - 9 January 1995

As can be seen from the table below our budget of 400 kECU over 3 years is divided in 4 activities: 225 kECU for the Network working groups which fund collaborative visits (secondements) and workshops, 80 kECU for the Network Conference scheduled for September 18-21, 1996 in Schwabisch Gmund (Germany), 60 kECU for Network support by the scientific secretary Dr. Z.Szotek (based in Daresbury Laboratory) and 35 kECU for the biyearly Network Management Meetings.
In this tablel one can also see the present state of our budget. All the numbers quoted are in kECUs.

Summary of Financial Position on January 27, 1995

	spent	Maximum
Working Groups	49.6	225
Conference		80
Network Support	16.0	60
NMB Meetings	15.6	35
Total	81.2	400

News from the Working Groups

Report on collaborative visit of S. Simak (Rennes) to M. Springborg (Konstanz), 26 November-11 December 1994

The problem which I should solve is the problem of dimerisation in TTF-BA crystals. A possible way to do it is to investigate the electronic properties and structure of TTF-BA using the powerful method FP-LMTO (full-potential version of the linear muffin-tin orbitals method).
A colloborative visit to Konstanz was devoted to work with the last version of the FP-LMTO program written by M.Springborg.

The main aims of the visit were:
1) to learn to work with the program under leadership of its author;
2) to calculate the structure of transpolyacetilene which is a good test-system;
3) to make adaptation of the program for calculation of the properties of TTF-BA.

The results of the visit are the following:
1) I can manage to work with the program by myself;
2) I have calculated the properties of transpolyacetilene and the results which I have got are in good agreement with the experiment and other calculations;
3) Under leadership of M.Springborg I have done required changes in the program to be able to investigate the dimerisation in TTF-BA.

So it was a very useful visit and its results should help me to solve the problem which I have.

As I could find a lodging in the Humboldt Institut in Konstanz the amount I had received from the network for the travel (train : economic class) and per-diem subsistance covered all my expenses.

Sergei Simak

Report on Green Function Working Group One day discussion on Dielectric Response

University of Nijmegen, Nijmegen, The Netherlands
(16 December 1994)

Attended by:
C. Patterson and D. Herrendorfer (*Univ. of Dublin*)
J. Inglesfield, M. Nekovee, G.P.M. Poppe (*Univ. of Nijmegen*)
E. Van Leeuken and R de Groot (*Univ. of Nijmegen*)
C.M.J. Wijers and P. de Boeij (*Univ. of Twente*)
V. Van Doren (*Antwerp*)
J. Michiels (*Groningen*)

The meeting consisted of informal talks given by the groups represented, followed by discussion. The talks were entitled:

Bond models for dielectric response: reflectance anisotropy of Si(001) 2x1 As (Dublin)
Methods for calculating local polarisabilities of semiconductors (Twente)
Simple models for calculating screened response (Groningen)
Dielectric functions for solids (Antwerp)
Dielectric response of a jellium solid with a simple periodic potential (Nijmegen)

The groups at Twente and Dublin are working in very closely related areas and each has an expertise which would benefit the other. The groups will undertake some collaborative work, hopefully under the auspices of the network.

C. Patterson and J. Inglesfield

Report on Taormina Workshop on Parallel Algorithms for Large System

by Beniamino Ginatempo, Dipartimento di Fisica, Università di Messina, ITALY

On November 26th-27th in Taormina (Sicily) we had an enjoyable and relaxing Workshop on *Parallel Algorithms for Large Systems.* The organizers were: Ezio Bruno, Sandro Giuliano,Walter Temmerman and myself. The audience consisted of 28 participants. There were 9 invited talks and 11 contributed talks whose abstracts, listed in alphabetic order of the speakers, are enclosed below. In my view it was quite a fruitful meeting and I would like to have the chance of making it a periodic rendez-vous of networkers. The expenses were covered by the Network and by the contributions from the Taormina City Council and Regione Siciliana.

The purpose of the workshop was not only to present the actual results obtained recently by means of parallelization of some of the most important algorithms and techniques, but also to discuss new ideas and possible applications of current problems of parallel computing, and to try to understand a little deeper what parallel computers can offer to condensed matter physicists.

On Saturday 26th the main topic was the Car-Parrinello method and the possibilities of parallelization offered by this algorithm. The invited talks on this subject were by: Ari P. Seitsonen (Helsinki and Berlin), Josè L. Martins(Lisboa), Simonetta Iarlori and Giacomo Fiumara (IBM-ECSEC, Rome), Alessandro De Vita (Lausanne) and Bjork Hammer (Lyngby). Mike Fearn (invited speaker from Oxford) talked about Bond Order Potentials. Contributed talks were by Hermann Winter (Karlsruhe), Guang Y. Guo (Daresbury) on response functions and magneto-crystalline anisotropy, respectively.

On Sunday 27th the main subject was the Multiple Scattering Theory with the invited talks by Rudy Zeller (Jülich) and G. Malcolm Stocks (Oak Ridge) on the application of KKR and real space Multiple Scattering calculations on Massively Parallel Computers, in particular, the Intel Paragon. Both speakers, apart from their results, discussed the machine related software problems, and the way they solved them. Contributed talks on various subjects were given by Balazs Újfalussy (Budapest and Vienna), Wolfgang Hierse (Darmstadt), Paul Miller (Bristol), Hugues Dreysse (Strasbourg), Walter M. Temmerman (Daresbury), Ezio Bruno (Messina), L. Puccio (Messina), Jos M. Thjissen (Njimegen) and B. Ginatempo (Messina).

Electronic Topological Transitions in Random Alloys

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ABSTRACT. Notwithstanding the substitutional disorder, the Fermi Surface of metallic alloys can be measured and computed. It may be defined as the locus of the peaks of the Bloch Spectral Function (BSF). Such Fermi surfaces, on varying the atomic concentrations, may undergo changes of their topology, known as Electronic Topological Transitions (ETT). Thus, for instance, pockets

of electrons or holes may appear or disappear, necks may open or close. ETTs cause anomalous behaviours of thermodynamic, transport and elastic properties of metals and constitute a fascinating field in the study of Fermi liquid systems. Although ETTs could be studied on pure systems as a function of the thermodynamic variables, nevertheless such a study would often require extreme experimental conditions. On the other hand, it is possible to explore the variations of atomic concentration, i.e. the valence electron per atom ratio, in metallic solid solutions with a relative experimental ease.

The theoretical determination of Fermi surfaces in metallic solid solutions

within the KKR-CPA framework and some examples ETT related phenomena will be briefly discussed. Moreover, the Fermi surfaces of several random alloys, calculated using the LDA-KKR-CPA theory, will be discussed in connection with experimental data. Namely, it will be shown that ab initio electronic structure calculations, for the studied systems, actually find changes in the Fermi Surface topology at those concentrations at which experiments report anomalous behaviours in thermodynamic and transport properties.

Electronic Structure Calculations and Molecular Dynamics Simulations on Massively Parallel Computers

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ABSTRACT. In the last few years the use of massively parallel computers to perform DFT-based electronic structure calculations and molecular dynamics simulations has proved to be a competitive alternative to standard vectorial supercomputing. After a pioneeristic stage in which the original analysis of the possible porting strategies was formulated and implemented [1], progress has been made by extending the approach to various algorithms, and due to the availability of more powerful and reliable parallel computers. We firstly review some work done involving different implementations of electronic structure based quantum molecular dynamics schemes. Secondly, we provide an analysis of the standard Car-Parrinello algorithm's [2] data structures which leads to a porting strategy suitable for the current generation of course-grained MIMDI machines. Implementation features, code optimisation and code performance will be discussed. Results from a recently completed production application on a large carbon system will be presented.

Use of SIMD machines in cluster problems

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ABSTRACT. Results are presented for the MasPar MP-1 (DECmpp 12000) series of computers which possess a single-instruction multiple-data (SIMD) architecture with processors arranged in a two-dimensional mesh. Two examples will be addressed. Many-body potentials proposed in the

literature have been used to perform simulations of fullerenes and Si-clusters [1]. The difficulty of attaining the absolute minimum for large clusters is discussed. Although parallelization does lead to a considerable speed-up compared to sequential codes, the determination of the ground state remains impossible for large clusters. Fragmentation of transition metal clusters at finite temperature due to a high-energy excitation has been studied by molecular dynamics and Monte Carlo simulations [2]. The process is found to be cahotic, with high sensistivity to inital conditions and the fragment distribution is consistent with power-law behavior.

[1] K.M. Nelson, C.F. Cornwell and L.T. Wille, Comp. Mat. Sci. (1994)
[2] L.T. Wille and H. Dreysse , Comp. Mat. Sci. 2 (1994) 519

Parallelisation of the Oxford Bond Order Potential (BOP) Program

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ABSTRACT. Recently, a novel angular-dependent interatomic potential for atomistic simulations of covalently bonded systems has been developed [1]. This so-called Bond Order Potential (BOP) has been rigorously derived within the two-center Tight Binding approximation and accounts for the directional bonding in materials such as sp-valent Si and C and d-valent transtion metals such as Nb and Ti. Morever, the many atom expansion for the BOP has been shown to be not only exact but also rapidly convergent [2]. Importantly, the BOP formalism is an O(N) method, the computational effort growing only linearly with the system size N. It is, therefore, significantly faster when applied to large systems than methods using direct diagonalization of the tight-binding Hamiltonain matrix where the time scales as the third power of the number of atoms N in the cell.

A substantial serial computer code has been developed at Oxford which performs atomistic simulations employing bond order potentials. This code has now been parallelised using the popular and portable PVM communications library.

In this talk we give an overview of the concepts underlying the derivation of bond order potentials plus a description of their evaluation. Some preliminary results of interfaces and defects are then presented. We go on to show how the code has been succesfully parallelised using a spatial decomposition strategy. The observed speedup, on adding processors, is shown to be near linear.

[1] D.G. Pettifor, Phys. Rev. Lett. **63**, p. 2480 (1989).
[2] M. Aoki, Phys. Rev. Lett. **71**, p. 3842 (1993).

Parallel Implementation of Ab-Initio Molecular Dynamics on a distributed enviroment

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[b]*IBM-ECSEC Roma, ITALY*

ABSTRACT. We present a parallel distributed memory implementation of an AB INITIO molecular dynamics code based on the Car-Parrinello (CP) method, for the study of the electronic and thermodynamical properties of condensed matter systems. The scheme combines the molecular dynamics (MD) technique for the computation of the statistical properties with the first-principle treatment of the interatomic forces through Density Functional Theory (DFT). We have implemented a parallel version of the CP method for a distributed architecture using the AIX PVMe software, which is an enhanced version of the standard PVM. The results presented here were obtained on a small cluster of IBM RISC workstations and on a IBM SP1 parallel architecture. In the distributed enviroment we parallelize the execution of the entire Molecular Dynamics loop for the electronic states of a realistic system. Even if the CP algorithm exhibits a complex communication pattern between the different nodes, we have achieved a good performance that is scalable almost linearly with the number of processors. We have realized a distribution on the different nodes of the total memory required to run the parallel simulation. This way we have overcome the bottleneck of large scale simulations which are characterized by huge memory requirements.

KKR-CPA calculations by PVM on a cluster under normal loading conditions

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ABSTRACT. We present an analisys of performances of a KKR-CPA code in a cluster of 6, FDDI connected, IBM/RISC 6000 mod. 580 computers, implemented to exploit the parallel nature of the KKR algorithm. That was realized (i) by studying a "normal" problem (the ab initio calculation of the electronic structure of a Cr-V alloy) and (ii) in normal loading conditions for the machines. The results, of course, have only a very low interest for the computer scientist, but have some relevance for the physicist using the cluster, which is interested more on wallclock times than performances. From such an analisys, we conclude that for the "small" problem at hand the hardware, PVM and a couple of tricks used can do a good job.

Magneto-crystalline Anisotropy Energy Calculation using Massively Parallel Computers

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ABSTRACT. Understanding the magneto-crystalline anisotropy of a magnetic solid is important both fundamentally and technologically. The first-principles calculation of the magneto-crystalline anisotropy energy is now possible, thanks to the development of the spin-polarized, relativistic band theory and to the power of the modern computers. Nevertheless, there is no rule of thumb yet and material specific calculations have to be performed. For complex systems such as magnetic multilayers, the magneto-crystalline anisotropy energy calculation is very computer-time consuming.

In this talk, I'll describe our band theoretical study of the magneto-crystalline anisotropy energy using the massively parallel computer Intel i860 hypercube at Daresbury.

Dissociation of H_2 on metal and alloy surfaces. [1]

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ABSTRACT. Total energy calculations are presented for the dissociative adsorption of H_2 on the surfaces of a noble metal, Cu, and an ordered alloy, NiAl (CsCl structure). The dissociation is activated on both surfaces, and the height of the activation barrier vary substantially with the H_2 impact parameters.

The variation in the barrier height for the H_2/Cu(111) is considered in detail and pieces of the full 6D potential energy surface are presented. The barrier variation is found to correlate strongly with the corrugation in the chemisorption energy of atomic hydrogen over Cu(111). The atomic positions of the *as-dissociated* H_2 thus determine to a large extend the degree of barrier variation.

Also a large degree of barrier variation is found on the NiAl(110) surface. This is the case even when the atomic positions of the *as-dissociated* H_2 are invariant. A detailed study of the electronic density of states projected onto atomic orbitals at the adsorbate and substrate positions reveals that the barrier variation originates from the presence of the *completely filled* Al(*3p*)-Ni(*3d*)-band. Over Ni-sites a strong hybridization between the *d*-states and the molecular anti-bonding state lowers the barrier for dissociation relative to the barrier over Al-sites.

Nearly self-consistent electronic structure for large systems: Parallel O(N) algorithm based on transferable localized orbitals

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ABSTRACT. We present an electronic structure method based on the use of highly localized, non-orthogonal (bond) orbitals that are transferable between chemically similar environments. This transferability is used to obtain nearly self-consistent electronic structure for large systems. The only quantity to be recomputed is an approximate inverse of the overlap matrix of the localized orbitals. A parallel implementation of this large sparse-matrix inversion is described.

Functionality and Applications of the AIMD Package

Simonetta IARLORI, F. BUDA, S. PATARNELLO
IBM-ECSEC Roma, ITALY

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[1] Work supported by the Danish Research Councils

ABSTRACT. We present the status of the development of the AIMD package, a simulation environment based on Ab Initio Molecular Dynamics method.

The primary goal of this package is to provide an advanced, and yet easy to use, computational tool to academic and industry researchers who want to approach ab initio molecular dynamics schemes and are not yet familiar with such framework.

AIMD is based on the density-functional theory using first principles pseudopotentials and a plane-wave basis set to describe the electronic wavefunctions. Different types of pseudopotentials are incorporated in the code, including "supersoft" pseudopotentials. This allows to treat a wide variety of compounds including first-row elements and transition metals. Available gradient-correction schemes are also implemented. The AIMD package allows to perform both microcanonical and canonical Molecular Dynamics simulations.

The project greatly benefits of the cooperation and experience of the IBM Research Division (Zurich Laboratory), where many of the techniques described above have been developed and deeply analysed in the context of several research projects.

Ongoing applications (metallocene catalysed ethylene polymerisation[1]) of the AIMD package will be presented.

[1] R.J. Meier, G.H.J. van Doremaele, S. Iarlori, F. Buda, J. of the Amer. Chem. Soc., in print.

First Principles Molecular Dynamics with Pseudopotentials

José Luís Martins
Departamento de Física, Instituto Superior Técnico
and INESC, Lisboa, PORTUGAL

ABSTRACT. In first principles molecular dynamics simulations the electronic structure is recalculated at each molecular dynamics step. A simulation may take several days in a dedicated workstation, and is therefore one of the problems that would benefit from parallel computers.

Currently first principles molecular dynamics is mainly (but not exclusively) associated with the pseudopotential plane-wave method of electronic structure theory. Existing codes are quite large, but most of the computing time is concentrated on performing standard numerical analysis operations, namely a three dimensional Fast Fourier Transform and matrix multiplication. By using BLAS subroutines and an interface subroutine for Fast Fourier Transforms, one can have a code that runs on any computer and still have a reasonable degree of paralellism in machines with a good vendor-supplied mathematical library. This strategy was used in a 4-processor Cray-2 machine resulting in wall-clock time smaller than the CPU time in conditions of moderate load but still with several processes competing for the CPU time.

The above strategy is only interesting for a distributed memory machine with a moderate number of processors. However the program was originally optimized for vectorization, when the parallel subroutines were not yet available. Once Cray supplied the parallelizing versions the program started running in parallel without a single new line of code.

For machines with a large number of processors, it may be interesting to design an algorithm with parallel machines in mind. Using grid methods is a way of avoiding the highly non-local

structure of the three dimensional Fast Fourier Transform used in plane-wave methods.

Parallel Solution of the Vortex Lattice by Recursion

Paul MILLER
H.H. Wills Physics Laboratory, University of Bristol, Tyndall Ave., Bristol BS8 1TL, U.K

ABSTRACT. The microscopic (Bogoliubov - de Gennes) equations are solved fully self-consistently for a superconductor in a magnetic field in the vortex state, with currents and fields also determined self-consistently via Maxwell's equations. The recursion method, a real space approach of O(N), is used to calculate Green's functions associated with each crystal lattice site in a vortex cell. Each site is allocated to a separate node of a parallel supercomputer for the calculations of electron number, order parameter and currents. A minimal communication between the nodes is required - only between iterations - so the method is well-suited to parallelization. The solutions have given new insight to the nature of Landau quantization in the vortex state.

Real space electronic structure calculations: combination of the finite difference and conjugate gradient methods

Ari P. SEITSONEN[a,b], M.J. PUSKA[b] and Risto M. NIEMINEN[b]
[a]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin-Dahlem, GERMANY*
[b]*Laboratory of Physics, Helsinki University of Technology, 02150 Espoo, FINLAND*

ABSTRACT. We discuss a scheme for a rapid solution of the eigenstates and the eigenenergies of the three-dimensional Schrödinger equation. The Hamiltonian operator is discretized on a point grid using the finite difference method. The eigenstates are searched for as a constrained (due to the orthogonality requirement) optimisation problem for the eigenenergies. This search is performed by the conjugate gradient method. We demonstrate the scheme by solving for the self-consistent electronic structure of the diatomic molecule P_2. Moreover, we demonstrate the efficiency of the scheme over the traditional Kimball-Shortley scheme by calculating positron states in low-symmetry solids. Also we describe the inclusion of this scheme to a self consistent calculation of positron in solids, and we discuss some preliminary results and possible ways of parallelising the methods above.

Parallel algorithms for the image restoration problem

Luigia PUCCIO
Dipartimento di Matematica, Università di Messina, ITALY

ABSTRACT. Parallel algorithms are proposed for the image restoration problem. The fundamental model describing this problem is given by a Fredholm integral equation of the first kind. In a first algorithm, without restrictions on the point spread function, we found its solution in a finite

dimensional spline space using Tikhonov polynomial regularization to minimize the ill-position of this operator equation.In this algorithm, there are two stages which have a high computation cost. They are: (1) the computing of the normal equation for the least squares image restoration and its regularized solution; (2) the choice of the optimum regularization parameter with an iterative scheme, the convergence of which is obtained in few iteration steps, but each iteration implies the solution of the above large dimension linear system. For these two stages, we consider parallel solution techniques, which are appropriate for a shared memory multiprocessor such as CRAY Y-MP 8/432 [4]. For distributed memory multiprocessor, as hypercube iPCS/2, a new fully asynchronous parallel algorithm has been proposed based on a "weighted domain decompositio" strategy [1], [2]. Actually the solution of this operator equation is found by means an efficient parallel wavelet packet matrix decomposition [3]. It is easily construct coarse grained parallel algorithms where the arithmetic work-load is very well balanced and which reach good efficiency on distributed memory multiprocessors as they require only very few nearest neighbour communications.

[1] L. BACCHELLI MONTEFUSCO and C. GUERRINI in, *Parallel Computing: Problems, Methods and Applications, P. Messina and A. Murli (eds.), Elsevier, (1991).*

[2] L. BACCHELLI MONTEFUSCO, C. GUERRINI and L. PUCCIO in Proceedings of *Curves and Surfaces, Chamonix, FRANCE, June 21st-27th 1990, Academic Press, Eds. P.J. Laurent, A. Le Mhaut L. L. Schumaker (1991), 321-324.*

[3] C.K. CHUI, L. MONTEFUSCO and L. PUCCIO (eds.), "Wavelets: Theory, Algorithms, and Applications" - Vol. V Series *Wavelets Analysis and its Applications - Academic Press (1994).*

[4] L.PUCCIO and D. LAZZARO in, *Parallel Computing: Problems, Methods and Applications, P. Messina and A. Murli (eds.), Elsevier, (1991), 379-387.*

Parallel Implementation of an O[N] Multiple Scattering Method: Applications to Metallic Alloys [1]

G. Malcolm STOCKS[a], D. M. C. NICHOLSON[a], Y. WANG[a], W.A. SHELTON, Z.SZOTEK[b] and W. M. TEMMERMAN[b]
[a] *Oak Ridge National Laboratory, USA*
[b] SERC, Daresbury,UK

ABSTRACT. A new approach to calculating the properties of complex systems within the local density approximation (LDA) that offers scalability on massively parallel supercomputers is outlined. The electronic structure problem is formulated in real space using multiple scattering theory. The standard LDA algorithm is divided into two parts. Firstly, finding the self-consistent field (SCF) electron density, Secondly, calculating the energy corresponding to the SCF density. We show, at least for metals and alloys, that the former problem is easily solved using real space methods. For the second we take advantage of the variational properties of a finite temperature generalized Harris-Foulkes free energy functional, a new conduction band Fermi function, and a

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[1] Work sponsored by Division of Materials Science and Applied Mathematical Sciences Program, Office of Basic Energy Sciences, USDOE, under contract DEAC05-84OR21400 with Martin Marietta Energy Systems, Inc.

fictitious finite electron temperature that, again, allow us to use real-space methods. Using a *compute-node* $\Rightarrow$ *atom* equivalence the new method is naturally highly parallel and leads to $O(N)$ scaling. We show scaling data gathered on the Intel XP/S 35 Paragon for systems up to 512-atoms/simulation cell. The new method is used to study the energetics of random and short ranged ordered solid solution alloys based on large supercell calculations. We comment on the role of charge inhomogenieties in determining the energetics of random alloys. We also show results of a large unit cell simulation of ferromagnetic NiCu alloys that show the importance of local moment inhomogenieties in the formation of magnetism in this alloy system.

Parallelization of the DF codes for superconductors

Walter M. TEMMERMAN
Daresbury Laboratory, Warrington WA4 4AD, UK

ABSTRACT. In this talk I will review the application of the Bogoliubov-de Gennes Density Functional theory to Nb and YBCO compounds. In particular I will discuss the implementation of the above in the LMTO-ASA bandtheory scheme which allows us to calculate materials specific electronic and superconducting properties on equal footing. Parallelization strategies will be discussed and results on the Intel i860 will be presented.

Embedding muffin tins into a finite difference grid

Jos M.THIJSSEN and J.E.INGLESFIELD
Physics Dept.- University of Nijmegen - THE NETHERLANDS

ABSTRACT. An order(N) method for the calculation of electronic structure is described. The method uses muffin tins which are embedded in a finite difference grid, allowing for a full potential treatment while keeping the number of grid points within reasonable bounds. Within the muffin tins, standard numerical techniques are used to integrate the Schoedinger equation. These solutions are then matched onto the finite difference grid, resulting in an embedding potential coupling the grid points lying just outside the sphere. Since the method is space-like, it is geometrically flexible and also suitable for parallel architectures. A tight binding method coupling nearest neighbour atoms (instead of finite difference grid points) will be discussed. It is based on the embedded muffin-tin method and uses a basis with zero-derivative boundary conditions on unit cell boundaries. This tight-binding method has the advantage of leading to an energy dependent Hamiltonian, which however looses some of its sparseness.

Application of the generalised KKR scheme

Balazs ÚJFALUSSY[a,b], L. SZUNYOGH[a,c] and P. WEINBERGER[a]
[a] *Institute for Technical Electrochemistry, Technical University Vienna, AUSTRIA*
[b] *Research Institute for Solid State Physics, Hungarian Academy of Sciences, HUNGARY*
[c] *Institute of Physics,*
Technical University Budapest, HUNGARY

ABSTRACT. The basic ideas of the generalised KKR formalism is presented. It is shown that a suitable choice of the reference system leads to well localised structure constants, which in turn leads to an elegant and numerically appealing multiple scattering based theory of surfaces and interfaces. Some details of the implementation on parallel computers are also discussed and the power of the method is demonstrated by calculating self-consistent quantum-well states in Ag overlayers on Au

The ab initio calculation of response functions, a case for parallelization

Hermann WINTER
Kernforschungszentrum Karlsruhe INFP, P.O. Box 3640 D-76128 Karlsruhe, GERMANY

ABSTRACT. We discuss the numerical implications of a first principles method to evaluate charge- and spin-density correlation functions based on the LSDA in conjunction with the RPA. To this purpose the KKR bandstructure has to be known to high accuracy in a wide energy range. The Bloch state coefficients are requi red up to angular momenta l = 5 and the wave functions must be determined on a dense point mesh in the interstitial region. Furthermore, considerable numerical effort is required to set up and to solve the implied Bethe-Salpeter equations. We point out how parallelization may be employed to shorten the time consuming steps in these kind of calculations. Results for simple metals and transition metals and compounds are presented.

Experience with multiple-scattering (KKR) calculations on parallel computers

Rudolf ZELLER
Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, GERMANY

ABSTRACT. The Kohn-Korringa-Rostoker method (multiple-scattering technique) has recently been extended to allow for the use of the full general electronic potential. For a wide variety of situations like periodic crystals, disordered alloys, surfaces, crystals or surfaces with defects, and isolated atoms and molecules the method represents an accurate and efficient way to calculate the electronic structure. If formulated with Green functions instead of wave functions, most of the computational work is used to determine these Green functions at a mesh of complex energy points, typically 20 to 40 points are sufficient. This work can naturally be parallized on distributed memory machines. The implementation of the computer codes for ideal periodic crystals on the Intel iPSC/860 and Paragon XPS is described and expectations, problems and successes connected with using these machines are discussed.

2^{nd} CIRCULAR

SPIN-ORBIT INFLUENCED SPECTROSCOPIES OF MAGNETIC SOLIDS

a workshop funded by the ESF - network:
RELATIVISTIC EFFECTS IN HEAVY ELEMENT CHEMISTRY AND PHYSICS
(coord.: P. Pyykkö, Helsinki and B. Hess, Bonn)

and the EU-HCM - network:
AB INITIO (FROM ELECTRONIC STRUCTURE)
CALCULATION OF COMPLEX PROCESSES IN MATERIALS
(coord.: W. Temmerman, Daresbury)

at Herrsching (D), from 20^{th} - 23^{rd} April 1995

organized by H. Ebert and G. Schütz

The aim of the workshop is to bring together researchers from all over Europe active in the field of **Spin-orbit influenced spectroscopies of magnetic solids** and related topics to present and discuss their latest results and ideas. There will be several invited contributions (**see list below**) dealing with spin-polarisation of photo-electrons from para- and ferromagnets, core level spectroscopies, linear and circular magnetic dichroism, magneto-optical Kerr-effect as well as other closely related phenomena.

Further participants are welcome. They will have the opportunity to present own contributions either as a short oral talk or as a poster. All costs for travelling, accomodation and meals have to be covered by the participants themselves (participants coming from a node of the EU-HCM-network will be supported by the network). The costs for accomodation including meals at the guest house we booked are 130 DM per day.

All information on how to get to Herrsching (close to the famous monastry Andechs) will be sent at the beginning of the next year together with the final list of participants.

List of Invited Speakers follows!

Looking forward to seeing you in Herrsching.
With best regards

Hubert Ebert and Gisela Schütz

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Fax.: (0821) 59 77 - 4 11
Email: schuetz@phibm30c.physik.uni-augsburg.de

List of Invited Speakers

D. Arvanitis, Uppsala
An angle dependent MCXD study of Ni, Co and Fe on Cu(100); Experiment versus Theory

K. Baberschke, Berlin
MCXD of Ni and Co monolayers: Tc(d), magnetic moment(d)

M. S. S. Brooks, Karlsruhe
B. Johansson, Uppsala
Relativistic Effects in Actinides

C. Brouder, Paris
Multiple-scattering approach to magnetic EXAFS

P. Carra, Grenoble
Unified approach to near-edge X-ray phenomena

C. T. Chen, Murray Hill
Orbital and spin magnetic moments from soft-X-ray MCD

M. J. Cooper, Warwick
Spin and orbital moments in rare earth ferromagnetic compounds studied by Compton scattering

H. Ebert, München
Multiple scattering approach to magnetic dichroism in electron spectroscopy of transition metal systems

R. Feder, Duisburg
Magnetic Dichroism and Spin Polarization in Valence Band Photoemission

A. Fontaine, Orsay
Spin polarization of conduction electrons in metallic multilayers and intermetallic compunds from X-ray magnetic circular dichroism

G. Güntherodt, Aachen

Linear magnetic dichroism in the angular distribution of photoelectrons (LMDAD) from the valence bands of Co(0001) and Fe(110)

G.-Y. Guo, Daresbury

Band Theoretical Investigation of Circular Magnetic X-ray Dichroism Sum Rules for Magnetic Multilayers

B. L. Gyorffy, Bristol

Dichroism in X-ray Fluorescence

G. Kaindl, Berlin

Dichroism in photoemission from Lanthanide materials

E. Kisker, Düsseldorf

Angular Dependent Magnetic Dichroism in Core Level Photoemission

G. Krill, Orsay

Magnetic Circular X-ray Dichroism in RE/TM intermetallic compounds Role of the hybridization between 4f and the conduction electrons

J. Kübler, Darmstadt

Calculated magneto-optical properties of transition metals and their compounds

P. M. Oppeneer, Dresden

Spin-orbit transmission effects in the Kerr spectra of compounds: an ab initio study

G. Sawatzky, Groningen

Magnetic X-Ray dichroism in studies of both short and long range magnetic order in antiferromagnetica

C. M. Schneider, Berlin

Imaging of magnetic domains by means of magnetic dichroisms: magnetic spectro-microscopy

G. Schütz, Augsburg

Magnetic EXAFS

J. Schwitalla, München

Inclusion of electron core-hole interaction in the calculation of $L_{2,3}$ X-ray-spectra for early transiton metals

J. Stöhr, San Jose

Angle-Dependent XMCD - Probing the Microscopic Origin of Magnetic Anisotropy

G. van der Laan, Daresbury

Magnetic Ground State Properties and Angular Dependent Magnetic Dichroism in Core Level Photoemission

C. Vettier, Grenoble

Resonant magnetic X-ray scattering in 5f compounds **P. Weinberger**, Wien

Relativistic AES

D. Weller, San Jose

Magneto Optical Spectroscopy in strongly anisotropic systems: FePt and Co

WORKSHOP

Full-Potential LAPW calculations with the WIEN95 code

April 19-22, 1995
Technical University Vienna, Austria

First Announcement

This informal workshop is concerned with recent progress in density functional calculations using the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as embodied in the WIEN95 code. The new version has been developed and improved with the help of many users, especially in collaboration with the groups

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

The workshop will be divided into two parts:

For novice users (April 19-20)

- The LAPW method and the use of WIEN95 (an introduction)
- Hands on calculations with the new user-friendly code

For experienced users (April 21-22)

- New features of WIEN95
- Recent progress in force calculations
- The use of local orbitals
- Contributions by participants (results and applications using WIEN93/95)
- Hands-on calculations with the new user-friendly code

The emphasis is placed on an open and accurate discussion of the relative strengths of the various methodologies currently in use. Introductory talks will be given by:

K.Schwarz (*TU Vienna*)
P.Blaha (*TU Vienna*)
P.Dufek (TU Vienna)
B.Kohler (*FHI Berlin*)
M.Faehnle (*MPI Stuttgart*)
H.Krimmel (*MPI Stuttgart*)
C.Ambrosch (*Uni Graz*)

General Information

Conference site: The conference will take place at the Technical University in Vienna, Gumpendorferstr.1a (3rd floor). Computer terminals for 20 persons have been reserved.

Arrival: The workshop will start at 9 am on Tuesday (Thursday) for part I (II). Thus it is advised to arrive on April 18 (April 20, for part II).

Accomodation: The workshop starts directly after the Easter holidays. Therefore it is highly recommended to make hotel reservations as soon as possible.

MAKE YOUR OWN RESERVATION!

Below is a list of a few recommended hotels/accomodations with the prices quoted in Austrian Schillings per night and person.

Hotel	Address	Telephone	Price
Pensionhotel Schneider	A-1060 Vienna Getreidemarkt 5	+43-1-58838-0 +43-1-58838-212(Fax)	900
Hotel Drei Kronen	A-1040 Vienna Schleifmuehlg.25	+43-1-5873289 +43-1-5873289-11 (Fax)	600
Lehrerheim des Lehrervereins	A-1080 Vienna Langegasse 20-22	+43-1-403 23 580	350
Youth Hostel	A-1070 Vienna Myrthengasse 7	+43-1-523 63 16 +43-1-523 58 49 (Fax)	50

For further addresses contact the organizer.

Please register soon!

Participants are encouraged to submit contributions in the form of talks (posters).

Deadlines: **The enclosed pre-registration form should be mailed to:**

Prof. K. Schwarz
Technical University Vienna
Getreidemarkt 9/158
A-1060 Vienna Austria
Email: kschwarz@email.tuwien.ac.at
Fax: +43 (1) 5868 937
before 15th February 1995.

Name and first name:
Professional title:
Address:
Phone:
Fax:
Email:
I wish to attend in part I (April 19-20) yes/no
I wish to attend in part II (April 19-20) yes/no
Please send me further information ( )
I plan to offer a contribution ( )
prefer poster ( ) or oral ( )
Tentative title ....
....
I will be accompanied by .... persons.
Date and Signature

STUDY WEEKEND: 21 and 22 APRIL 1995, DARESBURY LABORATORY

The grazing incidence monochromator on station 6.1 at the SRS (based on the Miyake principle) is 21 years old. In its life it has been used on three different synchrotron radiation sources - NINA at Daresbury, TANTALUS at Wisconsin and SRS at Daresbury - and has provided the light source for hundreds of published papers, mostly in photoemission for surface science.

Daresbury Laboratory is hosting this Study Weekend to celebrate the history of this instrument, and to look to the future of vacuum ultraviolet spectroscopy for surface science. Photoemission and related spectroscopies will be among the most popular techniques for stations on the next generation of synchrotron radiation sources. This meeting will help to focus ideas for instrumentation and science on the Low Energy Source SINBAD, the proposed new UK VUV source.

Speakers from the UK and the USA will cover the history and current status of and possible future advances in surface science in the VUV around the world. Research on metal and semiconductor surfaces, atomic and molecular spectroscopy and new interferometric techniques will also be described.

Contributions are invited for an extensive poster session, with a prize on offer for the best poster. Papers will be refereed for publication in an issue of the Journal of Synchrotron Radiation. The meeting is being sponsored by Daresbury Laboratory, Fisons Instruments (Surface Science Division) and CCP3 - the Collaborative Computational Project in Surface Science.

For more details, contact the Conference Office, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD UK (tel: 01925 603235, fax: 01925 603195)

University of Cagliari – Department of Physics
Research Position in Condensed Matter Theory

The Condensed Matter Theory Group at the Physics Department of the University of Cagliari, Italy, invites applications for a temporary research position of 12 to 18 months.

⟹ General info ⟸

- **Required expertise:** density-functional-theory–based computational physics
- **Other requirements:** research experience comparable to a PhD
- **Citizenship:** Applicants may be citizens of any Country
- **Working language:** English
- **Working site:** Cagliari, Italy
- **Salary:** about Italian Lire 1.900.000 net/month ($\geq$ permanent lecturer salary)
- **Starting date:** mid 1995 (negotiable)

⟹ Computational and Scientific info ⟸

The work, to be performed on

- **Serial/vector:** 3 SunSPARC10 stations (5 processors), plus Cray C90 shares
- **Parallel:** Shares of 32-nodes SP2 and Cray T3D,

mostly in cooperation with Vincenzo Fiorentini, will concern the following:

- **Physics:** defects and interfaces of III-V nitrides; metal-insulator interfaces; structure and adsorption on metal surfaces.
- **Techniques:** massive parallelization of electronic structure codes.

⟹ Queries and/or applications ⟸

including CV, research interests statement, and publication list, should be addressed to

Dr. Vincenzo Fiorentini
Dipartimento di Scienze Fisiche – Università di Cagliari
via Ospedale 72, I-09124 CAGLIARI, Italy
fax +39 70 666126 phone +39 70 664770 ext.207
e-mail : `fiore@sparc10.unica.it`

EC POSTDOCTORAL FELLOWSHIP

A postdoctoral fellowship is readily available for a period of at least two months with the maximum determined by the closing date of the programme (end of Aug. '95), financed by the EC, within the Human Capital and Mobility programme:

"ENERGY PATHWAYS IN BOND MAKING AND BREAKING AT SURFACES"

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

Applicants must be residents of an EC state, except Greece, and move to Greece during the tenure of the fellowship. The fellowship amounts of 1000 ECU per month, and in addition the traveling expenses, health insurance, conference participation and publication expenses.

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

Hariton M. Polatoglou
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Fax: +30 31 206138
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UNIVERSITY OF CAMBRIDGE - DEPARTMENT OF PHYSICS
POSTDOCTORAL POSITIONS IN CONDENSED MATTER THEORY

The Theory of Condensed Matter group expects to appoint Postdoctoral Research Associates starting in approximately October 1995 in a number of the following fields:

- Quantum study of complex processes in solids by ab initio density-functional total energy and dynamic calculations (MCP, RJN, VH)
- Theory of structural phase transitions and atomic ordering (VH)
- Quantum Monte Carlo calculations for realistic systems (RJN)
- Ab initio computational many-body theory of solids (RWG)
- Quantum phase transitions (DEK)
- Electron localisation and quantum transport (DEK)
- Random growth processes (RCB)
- Theory of colloidal systems (RCB)

Initials denote *Prof. V. Heine and Drs. R.C. Ball, R.W. Godby, D.E. Khmelnitskii, R.J. Needs, and M.C. Payne, who would be happy to discuss possible projects (Tel. +44 223 337200; Fax +44 223 337356).* The appointments will be for one year in the first instance, normally extendable for at least one further year.

Applicants should write to Dr. R.W. Godby (ref. PDRA), Cavendish Laboratory, Madingley Rd., Cambridge CB3 0HE, U.K., preferably before 15th February 1995, clearly stating the fields in which they are interested. They should enclose a curriculum vitae, current preprints and a list of publications, and should arrange for two letters of reference to be sent. Applications should include two self-addressed labels or envelopes, and e-mail addresses should be given wherever possible.

Electronic structure, magnetic and Fermi-surface properties of UPd_2Al_3

L.M. Sandratskii and J. Kübler
Institut für Festkörperphysik, Technische Hochschule
D-64289 Darmstadt, Germany
P. Zahn and I. Mertig
Institut für Theoretische Physik, Technische Universität
D-01062 Dresden, Germany

Abstract

The electronic structure of the antiferromagnetic heavy-fermion superconductor UPd_2Al_3 is determined by means of selfconsistent density-functional calculations in the local approximation treating the U 5f states as band states. The magnetic moment is obtained in agreement with experiment as well as the observed magneto-crystalline anisotropy. State densities and the effects of hybridization and of different magnetic configurations are discussed in detail. The Fermi surface is determined and illustrated; it is compared with recent de Haas - van Alphen measurements and is found to explain the data satisfactorily.

(submitted to Phys. Rev. B)
Latex/poscript version can be obtained from:
dg5m@mad1.fkp.physik.th-darmstadt.de(L.Sandratskii)

Localized Excitons and Breaking of Chemical Bonds at III-V (110) Surfaces

Oleg Pankratov and Matthias Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany

Abstract

Electron-hole excitations in the surface bands of GaAs (110) are analyzed using constrained density-functional theory calculations. The results show that Frenkel-type autolocalized excitons are formed. The excitons induce a local surface unrelaxation which results in a strong exciton-exciton attraction and makes complexes of two or three electron-hole pairs more favorable than separate excitons. In such microscopic exciton "droplets" the electron density is mainly concentrated in the dangling orbital of a surface Ga atom whereas the holes are distributed over the bonds of this atom to its As neighbors thus weakening the bonding to the substrate. This finding suggests the microscopic mechanism of a laser-induced emission of neutral Ga atoms from GaAs and GaP (110) surfaces.

(Submitted to Phys. Rev. Lett.)
LATEX version can be obtained from: oleg@theo24.RZ-Berlin.MPG.DE

Formation and structural analysis of a surface alloy: Al (111)-(2x2)-Na

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E. Lundgren and J. N. Andersen
Department of Synchrotron Radtiation Research,
Institute of Physics, Lund University, S-223 62 Lund, Sweden
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Fritz-Haber-Institut der Max-Planck-Gesellschaft,
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Abstract

The Al (111)-(2×2)-Na phase formed by adsorption of one-half monolayer Na at 300 K is shown to be a *surface alloy.* Quantitative agreement is achieved between the results of structure determinations by low energy electron diffraction, surface extended x-ray adsorption fine structure, and total energy calculations. The first four layers of the structure are shown to consist of a Na-Al-Na sandwich on a reconstructed Al substrate layer. It is suggested that the formation of the structure involves surface steps as *sources* of Al atoms.

(To be published in Phys. Rev. Lett.)
Manuscripts can be obtained from: cts@theo21.RZ-Berlin.MPG.DE

Ab-initio Calculations of Energies and Self-Diffusion on Flat and Stepped Surfaces of Al and their Implications on Crystal Growth

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Abstract

Using density-functional theory we investigate several properties of Al (111), Al (100), Al (110), and stepped Al (111) surfaces. We report results of formation energies of surfaces, steps, adatoms, and vacancies. For the adsorption and diffusion of Al on flat regions of Al (111) surfaces we find the hcp site energetically slightly preferred over the fcc site. The energy barrier for self-diffusion on Al(111) is very low (0.04 eV). Coming close to one of the two sorts of close packed, monoatomic steps on Al (111), labeled according to their {111} and {100} micro-facets, Al adatoms experience an attraction of ≤ 0.1 eV already before direct contact with the edge of the step. This attraction has a range of several atomic spacings and is of electronic origin. Upon arrival at the lower step edge, the adatom attaches with no barrier at a low energy five-fold coordinated site. Coming from the upper terrace, it incorporates into the step by an atomic exchange process, which has a barrier below 0.1 eV for both sorts of close packed steps. The barrier for diffusion along the lower edge is 0.32 eV at the {100}-faceted step and 0.39 eV at the {111}-faceted step. Unexpectedly the latter diffusion process proceeds by an exchange mechanism. Diffusion by a very similar exchange mechanism is also found for the "easy" direction on the Al (110) surface, i. e., along the channels. We show that Al (110) is a model system for diffusion at the {111}-faceted step on Al (111) because of its very similar local geometry. Our results enable the estimate of temperature ranges for different modes of homoepitaxial growth on Al (111)...

(Submitted to Phys. Rev. B on 30. October 1994)
REVTEX version can be obtained from: scheffler@fhi-berlin.mpg.de

The interaction of a point charge with a metal surface: theory and calculations for (111), (100) and (110) aluminium surfaces

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Abstract

The asymptotic form of the image interaction is derived for a classical external point charge at a distance z_1 outside a periodic metallic surface, generalising to real metals the analytical result of Lang and Kohn for jellium. The centre of gravity z_c of the induced charge coincides with the position of the image plane z_0 in the limit of linear response. However, whereas z_c is shown to depend through non-linear response on the magnitude of the external charge q, z_0 is independent of q. We show that surface periodicity does not modulate z_0, but adds to the image interaction a periodic component decaying exponentially with z_1. In addition, the long-ranged effect of non-linearity on the interaction energy is a term attractive to a positive external charge and proportional to $q^3/(z_1 - z_0)^4$. We report first principles pseudopotential calculations of the interaction energy with three aluminium surfaces: (111), (100) and (110). A supercell geometry is used. A discrete classical model without adjustable parameters reproduces the effect of the surface periodicity on the image interaction at each of the three surfaces.

(submitted to Journal of Physics: Condensed Matter)
The Word 5.1 or hardcopy version can be obtained from
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Magnetic Behavior of Transition-Metal Impurities in Alkali-Earth Metals

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Abstract

We present density functional calculations within the local density approximation for all transition metal impurities in the divalent hosts Ca, Sr and Ba. Our results predict sizable moments, even for impurities of the 4d and 5d series, being only slightly smaller than the moments obtained in the corresponding alkali metals.

(Submitted to Physical Review B)
Manuscript is available from: Ru.Zeller@kfa-juelich.de

A First-Principles Study of Exchange Integrals in Magnetite

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Abstract

A method is presented to calculate ab-initio exchange constants and spin-wave excitations of multi-sublattice magnetic structures on the basis of total energy calculations of incommensurate magnetic structures. Here the exchange energies, the dispersion curves and the Curie temperature for magnetite (Fe3O4) are obtained within the spin-wave theory and compared with experimental results.

(submitted to Journal of Physics: Condensed Matter)
Preprints available from the authors.

Exploring Magnetism in Transition Metallic Alloys via their Atomic Short Range Order

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Abstract

We propose that measurements of atomic-short-range-order (ASRO) in metallic alloys be used to test models of spin fluctuations in the paramagnetic state of metallic magnets. To support the idea, we describe a theory for both magnetic correlations and ASRO in alloys from a 'first principles',electronic structure basis with an application to an iron-rich $Fe - Al$ alloy.

Submitted to Phys. Rev. Lett. on 11th January 1995.
LATEX manuscript can be obtained from mfling@uk.ac.warwick.weed

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Electronic structure of icosahedral Al-Pd-Mn alloys

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Abstract

We present calculations of the electronic structure of a hierarchy of rational approximants to icosahedral Al-Pd-Mn quasicrystals. A model for the atomic structure has been constructed via the projection method, using atomic surfaces appropriate to reproduce the diffraction patterns of the icosahedral phase. The electronic structure has been calculated selfconsistently in the local-density approximation using the linear-muffin-tin-orbital (LMTO) method and tight-binding LMTO techniques. We show that the electronic density of states of the higher-order approximants is characterized by a structure-induced pseudogap at the Fermi-level. However, unlike for most quasicrystals investigated so far, no corresponding pseudogap exists for the lowest-order approximants.

(J.Non-Cryst.Solids (in print))
Manuscript can be ontained from jhafner@tph.tuwien.ac.at

All-Electron, Linear-Response Theory of Local Environment Effects in Magnetic, Metallic Alloys and Multilayers.

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Abstract

We present a theoretical framework for describing atomic short-range order and its effect upon such quantities as magnetisation and hyperfine fields in magnetic alloys. All electronic effects are accurately described from a 'first-principles', density-functional formalism, within the restriction of a rigid, uniform lattice. These effects include the filling of the spin-polarised electronic states, Fermi-surface contributions, and the rearrangement of charge and changes to the magnetisation as the chemical composition of the alloy fluctuates. We have calculated the magneto-chemical response for bulk $Fe_{87}V_{13}$ and $Cr_{70}Fe_{30}$ magnetic alloys to compare to those obtained from spin-polarised neutron scattering experiments. We also show the utility of these response functions for investigating the changes in, e.g., the moments and hyperfine fields for multilayers with varying textures in the case of FeV.

Journal of Physics: Condensed Matter, in press, 1995.
LATEX manuscript can be obtained from mfling@uk.ac.warwick.weed

Structural Phase Transformation of Aluminum Arsenide

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Abstract

The electronic structure, the charge density and the total energy of $AlAs$ in the zincblende (B3), rocksalt (B1), and nickelarsenide ($B8_1$) structures are studied using first- principles self-consistent local density calculations in a plane wave basis employing soft non- local pseudopotentials. Contrary to most other III-V compounds upon applying pressure, $AlAs$ transforms to the metallic nickelarsenide structure at a calculated pressure of 13.2 GPa, to be compared with a recent experimental value of 7.0±5.0GPa. The volume reduction at the transformation is calculated to be 21.0% (experimental value is 17.1% at 7.0 GPA). The equilibrium lattice constant of the nickelarsenide structure is found to be a=3.705 $\dot{A}$ and c=5.795 $\dot{A}$. From this structure no transformation appears to be possibble to the rocksalt structure.

(to be published in the Proceedings of the International Conference on "The Physics of the Semiconductors", Vancouver (Canada), August 10-14, 1994)
Latex-file available from vandoren@ruca.ua.ac.be

Electronic structure in icosahedral Al-Cu-Li quasicrystals and approximant crystals

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Abstract

The electronic structure has been calculated for large approximant crystals (up to 51752 atoms in the periodically repeated cell) to icosahedral AlCuLi quasicrystals. The results show that a deep structure-induced pseudogap at the Fermi energy is a generic property of the quasicrystal and of its crystalline approximants. The physical mechanism for the formation of the gap is discussed on the basis of a quasiperiodic generalisation of the nearly-free-electron model.

(J.Phys.: Condens. Matter 6(1994) 6977)
Reprints available from jhafner@tph.tuwien.ac.at

Band Theoretical Study of the Fermi Surface of CeB6

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Abstract

Fully relativistic band structure calculations have been performed for CeB6 and preliminary results presented. The Fermi surface is obtained and the dHvA frequency of the alfa orbit is calculated. A good quantitative agreement with the experimental results suggests the importance of including both the spin-polarisation and spin-orbit coupling in the calculations.

(Physica B (in press)
Postscript version can be obtained from: M.Suvasini@sheffield.ac.uk

The influence of generalized gradient corrections to the LDA on predictions of structural phase stability: The Peierls distortion in As and Sb

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Abstract

The crystal structure and phase stability of the group-V elements As and Sb has been investigated by total-energy calculations within the local-density approximation (LDA), without and including generalized gradient corrections (GGC). We show that contrary to the case of the group-VI elements Se and Te, where the LDA predicts crystal structures that are much more isotropic than observed, for As and Sb the LDA leads to equilibrium structures in reasonable or even good agreement with experiment and describes the pressure-induced phase transition to a simple cubic structure in Sb (but not in As) very well. The GGC corrections show a tendency to overshoot and to do not improve agreement with experiment. In both cases the main effect of the GGC's is to add an isotropic pressure to the system, while the local electronic and bonding properties at constant volume remain unchanged.

(submitted to J. Phys.: Condensed Matter)
Manuscript can be obtained from jhafner@tph.tuwien.ac.at

Ab–initio calculation of the structural and electronic properties of carbon and boron nitride using ultrasoft pseudopotentials

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Abstract

We present ab–initio calculations of the structural, cohesive, and electronic properties of various polymorphic forms of carbon and boron nitride. Our calculations are based on ultrasoft pseudopotentials and a variational approach to the solution of the Kohn–Sham equations. Optimization of the atomic geometries is performed using total energy calculations and by minimizing the energy via a quasi–Newton quench using the Hellmann–Feynman forces. Special attention is devoted to the convergence of the results with respect to the plane–wave basis. The entire set of structural energy differences calculated in our work is in good agreement with the most accurate results obtained using a variety of different techniques — our results represent the first consistent set of data based all on the same potential. We show that the use of ultrasoft potentials allows to achieve accurate results with low cut–off energies (and hence small basis sets).

(Phys.Rev. B50(1994)15606)
Reprints available from jhafner@tph.tuwien.ac.at

Enhanced Magnetism in Amorphous Co–Y Alloys: An ab–initio Approach

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Abstract

The magnetic properties of Co–Y crystalline intermetallic compounds and amorphous alloys have been investigated using molecular–dynamics simulations of the amorphous structure (based on effective tight–binding–bond–forces) and selfconsistent spin–polarized electronic structure calculations (using the supercell approximation for the amorphous phases). We find that the amorphous structure is characterized by a rather strong chemical short–range order (stronger than in amorphous Fe–Y, but weaker than in Ni-Y alloys). As a consequence, the total electronic DOS is also similar in the crystalline and amorphous phases, apart from a smearing of the fine–structure characteristic for the long–range order in the intermetallic compounds. All crystalline $\mathrm{Co}_x\mathrm{Y}_{100-x}$ alloys with $x \geq 75$ and all amorphous alloys with $x \geq 45$ are ferrimagnetic. The Laves phase $\mathrm{Co_2Y}$ shows metamagnetism. The disorder-induced smearing of the electronic DOS eliminates the metamagnetic instability and is responsible for the increase of the paramagnetic DOS at the Fermi level and for the enhancement of magnetism. We find that the ferrimagnetic coupling, together with the strong tendency to hetero-coordination is important for the persistence of magnetic ordering in the Y–rich regime.

(Submitted to Phys.Rev. B)
Manuscript available from jhafner@tph.tuwien.ac.at

Structural and electronic properties of clean and hydrogenated diamond (100) surfaces

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Abstract

The structural and electronic properties of clean and hydrogenated diamond (100) surfaces have been investigated via fully selfconsistent ab-initio calculations. We find that the clean and the monohydrogenated surfaces reconstruct via the formation of rows of symmetric dimers. Further hydrogenation to a coverage of 1.5 monolayers stabilizes a surface with a (1x1) periodicity in the C-layers, albeit with a low H-desorption energy for the formation of of the reconstructed monohydride surface. The electronic properties of the surfaces have been calculated. Surface states within the bulk gap are found for the clean surface and for the strongly hydrogenated surface, but not in the monohydride case.

(Europhys.Lett. 28 (1994) 659)
Reprints available from jhafnr@tph.tuwien.ac.at

The "fuzzy" tight-binding Monte-Carlo method: A novel O(N)-technique for calculating structural and electronic properties of materials

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Abstract

We present a novel approach to computer-simulations of the structural and electronic properties of materials that scales linearily with the number of electrons in the system. The approach is based on two essential steps: (i) The introduction of a new "fuzzy" Monte Carlo technique based on the approximate calculation of the total energy of the system. We show that a statistical error in the energy may be included in the thermal distribution via a new formulation of the Glauber dynamics of the Monte Carlo method. (ii) The calculation of the total electronic density of states and total energy via a real-space recursion technique for a set of random initial states and a decomposition into local densities of states and individual atomic contributions to the total energy. Applications of the new technique to the simulation of liquid and amorphous carbon at different densities are presented.

(submitted to Phys.Rev.Lett.)
Manuscript obtainable from jhafner@tph.tuwien.ac.at

Disorder and non-collinear magnetism in permanent-magnet materials with the $ThMn_{12}$ structure

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Abstract

We report calculations of the non-collinear magnetic structures of $YFe_{12-x}Mo_x$ permanent-magnet materials, using a novel variant of a spin-polarized tight-binding–linear-muffin-tin-orbital (TB-LMTO) technique allowing for local spin-quantization axes on each site and considering spin-orbit coupling. The ternary $YFe_{12-x}Mo_x$ compounds crystallize in the tetragonal $ThMn_{12}$ structure which can be stabilized only by the partial substitution of Fe by an early transition metal like Mo. We show that the substitutional disorder breaks the equilibrium between ferro- and antiferromagnetic interactions among the iron atoms and leads to canted spin-structures at low Mo-content (x $\sim$ 1) and to spin-glass-like behaviour at higher Mo-content (x $\sim$ 3). The results are in good agreement with Mössbauer and magnetization measurements.

(submitted to Phys. Rev. Lett.)
Manuscript obtainable from jhafner@tph.tuwien.ac.at

Ab initio electronic structure of a small bandgap polymer: poly-aminosquaraine

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Abstract

Poly-aminosquaraine is the prototype of a class of organic polymers which recently has been shown to provide a route towards small bandgap materials. We predict that poly-aminosquaraine has a small bandgap of ~ 0.5 eV. Our prediction is based upon a detailed analysis of first-principles calculations of the geometrical and the electronic structure, using the Car-Parrinello technique of simultaneous optimization. We analyse the bands around the Fermi level in terms of a simple tight-binding model based upon the highest occupied and lowest unoccupied states of the individual squaraine molecules. The small bandgap of the polymer is shown to be the result of the small splitting between the occupied and the unoccupied states of the squaraine molecule combined with a favourable hybridization in the polymer. It should be possible to analyze the electronic structure of a wide class of squaraine based polymers in the same way.

(to appear in J. Chem. Phys.,)
Manuscript available from: brocks@prl.philips.nl)

Coster-Kronig contributions to magnetic circular dichroism in the $L_{2,3}$ x-ray fluorescence of iron

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Abstract

High resolution x-ray fluorescence spectroscopy has been performed on magnetically oriented polycrystalline iron samples. Circularly polarized synchroton radiation was used to excite the Fe $L_{2,3}$ x-ray emission either directly from a bending magnet (white radiation) or from an asymmetric wiggler followed by a monochromator tuned to the L_2 edge. Large differences in the magnetic circular dichroism (MCD) were observed. Spin-polarized relativistic LMTO calculations and a simple qualitative model demonstrates that the L_3 x-ray emission dichroism is partially canceled by the L_2-$L_3M_{4,5}$ Coster-Kronig process. The Coster-Kronig process is large enough to make MCD x-ray absorption experiments, performed in the fluorescence mode, unreliable.

(Phys. Rev. B (Rapid Comm.) 51, 1370 (1995))
Manuscripts available from hague@ccr.jussieu.fr

Electronic Structure and Optical Properties of Si/Ge superlattices

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Abstract

A new approach that combines various calculational methods is presented for studying the effect of the Si-Ge interface onto the electronic and optical properties of $\mathrm{Si}_n\mathrm{Ge}_m$ superlattices (SL's). In particular our approach employs: (i) The Tight Binding, (TB), method to calculate the band structure of the $\mathrm{Si}_n\mathrm{Ge}_m$ SL's which exhibit an abrupt or diffused Si-Ge interface (ii) The Coherent Potential Approximation (CPA) method, in order to describe the interdiffusion across the Si-Ge interface and finally (iii) The Cubo-Greenwood formula in order to obtain the optical absorption coefficient of the SL. This approach is applied on a strained symmetrized $\mathrm{Si}_5\mathrm{Ge}_5$ SL and our results confirm recent theoretical and experimental ones that support the finding that interdiffusion across the interface of the SL degrades the strength of the direct optical transitions. According to out findings this degrade is attributed to the widening of the energy gap of the SL that follows the interdiffusion. The present method is more accurate than others based on calculating transition matrix elements explicitly, because it incoprorates the effects of randomness through the CPA on both the density of states and the optical transition matrix elements.

(submitted to Europhysics Letters)
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The scaling of the Tight-Binding Hamiltonian

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Abstract

We reexamine the variation of the Slater-Koster Tight-Binding (SK-TB) parameters with the interatomic distance and the lattice structure. It is shown that when volume effects are separated from lattice (field) effects, the scaling with the volume can be described in terms of the electron density (or equivalently the parameter r_s) while the scaling with the lattice structure can be described in terms of the number of nearest neighbours. The proposed scaling form appears to fit very accurately SK-TB parameters of Si obtained by the TB-LMTO method.

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Electronic Structure and X-Ray Magnetic Dichroism in Random Substitutional Alloys containing f-Electron Elements

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Abstract

The KKR-CPA method combines multiple scattering theory and the coherent potential approximation to calculate the electronic structure of random substitutional alloys of transition metals. In this letter we describe the generalization of this theory to describe f-electron alloys. The theory is fully relativistic and spin-polarised. It is illustrated with the first calculation of the electronic structure and magnetic dichroism curves for a random substitutional alloy containing rare earth or actinide elements from first principles.

(Accepted for Publication: Phys Rev B.)
Manuscripts available from: pha05@cc.keele.ac.uk

Structural Analysis of the two c(2×2) Phases of Na Adsorbed on Al (100)

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Abstract

We have studied the adsorption of Na on Al(100) at different substrate temperatures using low-energy electron diffraction (LEED) and density-functional theory (DFT) calculations. Below 180 K and above 260 K well-ordered c(2×2) overlayers develop which are completely different in structure. As determined by the LEED intensity analysis the Na atoms in the phase formed at low temperature occupy fourfold hollow sites where the nearest-neighbour Na-Al bond length is 3.27 ± 0.01 Å. The Na atoms in the phase formed above 260 K occupy substitutional sites. For this structure the LEED intensity analysis shows a contraction of the topmost Al interlayer spacing of 9.1 ± 0.5 Å and a nearest-neighbour Na-Al bond length of 3.07 ± 0.01 Å. On heating, the low-temperature c(2×2) structure is irreversibly transformed into the room-temperature structure. The adsorption sites and accompanying substrate relaxations and/or reconstructions agree very closely with those predicted from DFT calculations.

(Submitted to Surf. Sci.)
Preprints can be obtained from: `cts@theo21.RZ-Berlin.MPG.DE`

The Interaction of Hydrogen with the (110) Surface of NiAl

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Abstract

The adsorption of hydrogen onto the (110) surface of the ordered alloy NiAl is being investigated experimentally and theoretically. At this stage, the experimental and theoretical results are complementary. Experiment reveals that the dissociative adsorption of atomic hydrogen is activated and indicates that the presence of H on the surface causes dramatic changes in the atomic positions of the Ni and Al atoms. Density functional theory for a (1×1) H overlayer identifies the H-bonding site as the Ni-Ni bridge and predicts the surface rippling on clean NiAl (110) is removed by hydrogen.

(Submitted to Surf. Sci.)
LATEX version can be obtained from: `aubrey@solid.ssd.ornl.gov`

Theory of alkali metal adsorption on close-packed metal surfaces

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Abstract

Results of recent density functional theory calculations for alkali metal adsorbates on close-packed metal surfaces are discussed. Single adatoms on the (111) surface of Al and Cu are studied with the self-consistent surface Green-function method by which the pure adsorbate-substrate interaction may be analyzed. Higher coverage ordered adlayers of K on Al (111), Na on Al (111), and Na on Al (001) are treated using the *ab-initio* pseudopotential plane wave method which affords the prediction of coverage dependent stable and metastable adsorbate geometries and phase transitions of the adsorbate layers. Together, these studies give insight and understanding into current key issues in alkali metal adsorption, namely, the nature of the adsorbate-substrate bond at low coverage and the occurrence of hitherto unanticipated adsorbate geometries, and the associated electronic properties.

(To be published in Surf. Rev. and Lett. (1995))

Copy can be obtained from: `cts@theo21.RZ-Berlin.MPG.DE`

Frustrated H-induced Instability of Mo (110)

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Abstract

The large interest in the properties of transition metal surfaces has been recently fostered by inelastic helium atom scattering experiments carried out by Hulpke and Lüdecke. Sharp and giant anomalies in the surface phonon dispersion curves along $\overline{\Gamma\mathrm{H}}$ and $\overline{\Gamma\mathrm{S}}$ have been detected on W (110) and Mo (110) at a coverage of one monolayer of hydrogen. At the same critical wave vectors a smaller second indentation is present in the experimental phonon branches. Recently we have proposed a possible interpretation which is able to explain this and other experiments. In this paper we discuss results of our recent ab initio calculations of the atomic and electronic properties of the clean and H-covered Mo (110) surface in more detail. For the full monolayer coverage the calculated Fermi-surface contours are characterized by strong nesting features which originate the observed anomalies.

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Ab-initio calculations of interaction energies of magnetic layers in noble metals: Co/Cu(100)

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Abstract

We present ab–initio calculations for the interlayer exchange coupling of magnetic Co(100) layers in Cu. The calculations are based on a KKR Green's function method for planar defects and apply the frozen potential approximation allowing a direct calculation of the interaction via single particle energies. Thus the subtraction of large total energies is avoided and efficient calculations for large layer thicknesses are enabled. By dividing the 2D Brillouinzone into areas around different stationary points $\mathbf{q}_i$, a clear analysis of the asymptotic behavior is given. The different dependences of the short and long oscillation periods on the thickness of the magnetic layers are explained by the $\mathbf{q}_{||}$- and symmetry projected DOS of the Co layers. The effects of roughness on the interlayer coupling are simulated, leading to a strong reduction of the amplitudes and a suppression of the short wavelength period. Our calculations are in good agreement with experiments and give a consistent picture of interlayer coupling in Co/Cu(100), as far as both the dependence on the thickness of the magnetic layers as well as the dependence on roughness is concerned.

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Fermi Surfaces and Electronic Topological Transitions in Metallic Random Alloys (I): the influence on equilibrium properties

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Abstract

In this paper we address the question of how the so-called Electronic Topological Transitions (ETT) can affect the physical properties of metallic random alloys, extending the existing theory in order to include substitutional disorder. The ETTs, or, as sometimes called, the Lifshitz 2 and 1/2 transitions, occur when the chemical potential passes through a Van Hove singularity on changing the thermodynamic state of a metal. That can be easily achieved by alloying. As a consequence, the Fermi Surface topology changes and a number of transport as well as equilibrium properties show anomalies, when studied vs. the concentration. We show that these anomalies might be slightly affected by disorder scattering and/or finite temperatures. Our theoretical results, which hold in a neighbourhood of the ETT, predict anomalies in correspondence of such variations of Fermi Surface connectivity for the equilibrium volume and enthalpy of mixing. In particular our theory predicts deviations of the alloy lattice parameter from the Vegards rule. These are confirmed by our ab initio KKR-CPA calculations for the Ag_cPd_{1-c} system. Detailed calculations of the Ag_cPd_{1-c} Fermi Surfaces are presented in a separate paper (II).

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Fermi Surfaces and Electronic Topological Transitions in Metallic Random Alloys (II): Ag_c-Pd_{1-c}

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Abstract

We calculated the Fermi Surfaces of Ag_c-Pd_{1-c} vs. Ag atomic concentration, within the fully relativistic Korringa-Kohn-Rostoker-Coherent-Potential-Approximation (KKR-CPA) framework. The Fermi Surfaces of these alloys changes, on varying the concentration, from the Pd-like to the Ag-like topology. This implies that a number of Electronic Topological Transitions (ETT) occur on changing the e/a ratio, as a consequence of the fact that the Fermi level moves away from the *d*-states towards the *sp*-states. It is well known that such changes in connectivity of the Fermi Surfaces affect transport coefficients, however as we have shown in I, also equilibrium properties such equilibrium volume, specific heat, enthalpy of mixing, etc. display anomalies at the same concentrations where such topological changes occur. In particular we have found 5 ETTs, in correspondence of the deviations from the Vegards law of the lattice parameter shown in I. Another unexpected result of this study is that, in the range of atomic concentration between 0.55 and 0.69, this alloy Fermi surface is simply connected, although non spherical, as a for simple metal. Moreover, we show that a fully relativistic study is necessary for AgPd Fermi Surfaces, because the Spin-Orbit interaction is responsible of the fact that the two hole pockets at X close at different concentrations.

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HIGHLIGHT OF THE MONTH FOLLOWS

Galvano-magnetic and magneto-optical properties of transition metal systems

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The abstracts collected in the last issues of this newsletter are a nice demonstration that within the *Network Community* there is considerable interest in the impact of relativistic effects on the electronic structure. Obviously, spin-orbit coupling plays a prominent role in magnetic solids because on one hand it gives rise to a large number of interesting phenomena and on the other it poses a big challenge to the basic formalism as well as implementation. The latter is caused by the demand that both spin-orbit coupling and magnetism have to be accounted for at the same time. The most advanced Hamiltonian, commonly used today, which meets this requirement is briefly described here. It is demonstrated for the conductivity tensor how simple symmetry considerations allow to predict the consequences of the interplay between spin-orbit coupling and magnetism. Recent calculations for the DC conductivity, Kerr-rotation and magnetic X-ray dichroism for various transition metal systems indicate that the above mentioned Hamiltonian supplies a sound basis for understanding all these phenomena giving (in general) a quantitative description of them.

3 Dirac Hamiltonian and band structure schemes

As already pointed out in 1973 by Rajagopal and Callaway, treating magnetism in a proper relativistic way, by extending the original Hohenberg-Kohn-Sham density formalism, leads to a current density formalism with the expectation value of the four-current density operator as the central quantity. Unfortunately, this approach seems to be – at least for the moment – too ambitious. Therefore, in order to describe relativistic effects and spontanous magnetism on an equal footing one has to use an extension of the non-relativistic spin-density-functional formalism in the form originally suggested by McDonald and Vosko [1]. The corresponding Dirac-Hamiltonian has the form:

$$\mathcal{H}_D = \frac{c}{i}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \frac{1}{2}(\beta - I) + V_H(\mathbf{r}) + \bar{V}_{xc}(\mathbf{r}) + V_{spin}(\mathbf{r}), \tag{1}$$

with α_i and β being the standard Dirac matrices and $V_H(\mathbf{r})$ the Hartree potential. The exchange correlation potential consists of a spin averaged- and a spin-dependent part, with the latter given by:

$$V_{spin}(\mathbf{r}) = \beta\boldsymbol{\sigma} \cdot \frac{\partial E_{xc}}{\partial \mathbf{m}}(\mathbf{r}) = \beta\boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{r}), \tag{2}$$

where $\mathbf{m}$ is the spin magnetisation density. Obviously, any explicit coupling to the orbital degree of freedom of the electrons is ignored in the potential terms of the above Hamiltonian, but it would be present in the framework of a more general current density functional formalism.

As demonstrated by Feder et al. [2] and Strange et al. [3], when dealing with an isolated spherically symmetric potential well (i.e. $V(\mathbf{r}) = V(r)$ and $\mathbf{B}(\mathbf{r}) = \mathbf{B}(r)$) the most important consequence of $V_{spin}(\mathbf{r})$ is that the solutions $\Psi_\Lambda(\mathbf{r}, E)$ of the above Hamiltonian have in general no unique spin angular character. Fortunately, the summation in

$$\Psi_\Lambda(\mathbf{r}, E) = \sum_{\Lambda'} \Psi_{\Lambda'\Lambda}(\mathbf{r}, E) = \sum_{\Lambda'} \begin{pmatrix} g_{\Lambda'\Lambda}(r, E)\, \chi_{\Lambda'}(\hat{\mathbf{r}}) \\ i f_{\Lambda'\Lambda}(r, E)\, \chi_{-\Lambda'}(\hat{\mathbf{r}}) \end{pmatrix}, \tag{3}$$

where $\chi_\Lambda(\hat{\mathbf{r}})$ are the spin-angular functions and $\pm\Lambda = (\pm\kappa, \mu)$ are relativistic quantum numbers, is restricted to $\mu' = \mu$ and $\kappa' = \kappa, -\kappa - 1$ (i.e. $p_{1/2,\mu} - p_{3/2,\mu}, d_{3/2,\mu} - d_{5/2,\mu}, \ldots$), which seems to be sufficient for all interesting cases.

Starting from $\Psi_\Lambda(\mathbf{r}, E)$ as the solution of the single site problem spin polarized relativistic (SPR) versions of the LMTO- and KKR-methods have been developed by various groups.

4 Symmetry considerations

A direct consequence of the Hamiltonian in Eq. (1) is that the symmetry of a system depends on the direction $\hat{\mathbf{M}}$ of its magnetisation $\mathbf{M}$ or equivalently on the direction of the effective magnetic field $\mathbf{B}$ in Eq. (2). Obviously, this also applies to the irreducible part of the Brillouin zone that is determined by the corresponding magnetic point group. Since symmetry imposes restrictions on the form of any equilibrium property tensor, again this will depend on $\hat{\mathbf{M}}$. Symmetry restrictions on transport property tensors have been discussed by Kleiner [4] in a general way. Here it is sufficient to consider the restrictions due to the Laue group which emerges from the magnetic space group by replacing every translation by the identity and every improper rotation by its proper counterpart.

For the frequency dependent conductivity tensor $\boldsymbol{\sigma}(\omega)$ of a cubic system one gets for example for $\hat{\mathbf{M}}[001]$:

$$\boldsymbol{\sigma}(\omega) = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix} \tag{4}$$

and for $\hat{\mathbf{M}}[110]$

$$\boldsymbol{\sigma}(\omega) = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{xx} & -\sigma_{xy} \\ -\sigma_{xz} & \sigma_{xz} & \sigma_{zz} \end{pmatrix} . \tag{5}$$

Here one should note that the reduction in symmetry due to the magnetisation that is manifested by Eqs. (4) and (5) occurs only if spin-orbit coupling is present. If one could switch off spin-orbit coupling for a spin-polarized system its properties would not depend anymore on the orientation of the magnetisation and for this reason its symmetry would be that of the corresponding paramagnetic state. Thus it is magnetisation together with spin-orbit coupling that leads to a symmetry reduction compared to the paramagnetic case. The extent to which this reduction in symmetry takes place is determined by the orientation of the magnetisation. However, whether the spin-orbit induced property is observable or not still depends on the magnitude of the magnetisation and the strength of the spin-orbit coupling.

5 Galvano-magnetic properties of disordered alloys

The dependence of the conductivity tensor $\boldsymbol{\sigma}(\omega = 0)$ on the spontanous magnetisation $\mathbf{M}$ of a system gives rise to the so-called galvano-magnetic phenomena. According to Eq. (4) the corresponding resistivity tensor $\boldsymbol{\rho} = \boldsymbol{\sigma}^{-1}$ for a cubic system with $\hat{\mathbf{M}}[001]$ has the form:

$$\boldsymbol{\rho} = \begin{pmatrix} \rho_{\perp} & -\rho_H & 0 \\ \rho_H & \rho_{\perp} & 0 \\ 0 & 0 & \rho_{||} \end{pmatrix} . \tag{6}$$

Obviously, the off-diagonal element ρ_H can be seen as a direct measure of the anomalous Hall resistivity (AHR). The so-called spontanous magneto-resistance anisotropy (SMA) on the other hand is defined as the ratio

$$\frac{\Delta\rho}{\bar{\rho}} = \frac{\rho_{||} - \rho_{\perp}}{\bar{\rho}}, \tag{7}$$

with the isotropic resistivity $\bar{\rho} = 1/3\,(2\rho_{\perp} + \rho_{||})$.

An adequate prescription for calculating the residual resistivity $\boldsymbol{\rho}$ of a disordered alloy system at $T = 0K$ or the corresponding conductivity $\boldsymbol{\sigma}$ is supplied by the Kubo-Greenwood-equation:

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi V_{\mathsf{cryst}}} \mathrm{Tr} \left\langle j_{\mu}\, \mathrm{Im}G^{+}(E_{\mathrm{F}})\, j_{\nu}\, \mathrm{Im}G^{+}(E_{\mathrm{F}}) \right\rangle_{\mathsf{conf.}} . \tag{8}$$

Here j_{μ} is the μ-th spatial component of the electronic current density operator $\mathbf{j}$, G^{+} is the single particle Greens function at the Fermi energy E_F and $< ... >_{\mathsf{conf.}}$ denotes the atomic configuration average for a disordered alloy.

Butler [5] has worked out in detail how this expression can be evaluated within the framework of the non-relativistic KKR-CPA formalism. As we have seen above the non-isotropic form of $\boldsymbol{\sigma}$ stems from the interplay of magnetism and spin-orbit coupling. Therefore, in order to account for galvano-magnetic effects Eq. (8) has to be evaluated within a relativistic framework. Accordingly, G^+ is:

$$\begin{aligned} G^+(\mathbf{r},\mathbf{r}',E) &= \sum_{\Lambda\Lambda'} Z_\Lambda(\mathbf{r},E)\,\tau_{\Lambda\Lambda'}(E)\,Z^\times_{\Lambda'}(\mathbf{r}',E) \\ &- \sum_{\Lambda} Z_\Lambda(\mathbf{r}_<,E)\,J^\times_\Lambda(\mathbf{r}_>,E), \end{aligned} \tag{9}$$

with $\tau_{\Lambda\Lambda'}$ the scattering path operator and Z_Λ (J_Λ) the regular (irregular) solution of the single-site Dirac equation (see Eq. (1)) normalized according to the scattering theory.

The proper relativistic form for the current density operator $\mathbf{j}$ is $ec\boldsymbol{\alpha}$. However, when using this expression in the atomic sphere approximation (ASA) the electronic wavefunction in the interstitial region may not be accurate enough. This problem can be circumvented by using one of the following transformations of the matrix elements

$$\begin{aligned} < \phi_\Lambda(E)|\boldsymbol{\alpha}\cdot\mathbf{a}_\lambda|\phi_{\Lambda'}(E')> &= \frac{2c}{c^2+E+E'} < \phi_\Lambda(E)|\frac{1}{i}\boldsymbol{\nabla}\cdot\mathbf{a}_\lambda \\ &\qquad + \frac{v}{c}\boldsymbol{\alpha}\cdot\mathbf{a}_\lambda - \frac{B}{c}i\beta(\boldsymbol{\alpha}\times\mathbf{a}_\lambda)_z\,|\phi_{\Lambda'}(E')> \qquad (10) \\ &= \frac{2}{(E+c^2/2)^2-(E'+c^2/2)^2} \qquad (11) \\ &\quad \times\Big[ic < \phi_\Lambda(E)|\boldsymbol{\nabla}V\cdot\mathbf{a}_\lambda + \beta\sigma_z\boldsymbol{\nabla}B\cdot\mathbf{a}_\lambda|\phi_{\Lambda'}(E')> \\ &\quad -(E-E') < \phi_\Lambda(E)|V\boldsymbol{\alpha}\cdot\mathbf{a}_\lambda - iB\beta\sigma_z(\boldsymbol{\alpha}\times\mathbf{a}_\lambda)_z|\phi_{\Lambda'}(E')>\Big]\,, \end{aligned}$$

with $\mathbf{a}_\lambda$ being a polarisation vector and $\mathbf{B} = B\,\hat{\mathbf{z}}$ has been assumed.

The above scheme has recently been applied for the first time to the *fcc*-alloy system $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ [6]. This system was chosen because it possesses one of the highest SMA and is therefore of considerable technological importance. As Fig. 1 shows, the calculations reproduce satisfactorily the variation of the SMA with concentration. The most important reason for the much higher theoretical values compared with experiment seems to be the fact that the calculated isotropic resistivity $\bar{\rho}$ (not shown here) is to the same extent smaller than the experimental one. This is not unexpected because our calculations account only for the contribution to $\bar{\rho}$ due to scattering events caused by chemical disorder; any other sources such as e.g. short range order or grain boundaries are ignored.

In addition one should note that the calculations have been performed for $\hat{\mathbf{M}}[001]$ while the experimental data are for polycrystaline samples. However, as can be seen from measurements on single crystals, this contributes only neglegibley to the deviation in Fig. 1.

In Fig. 1 results for the AHR are given in terms of the so-called Hall angle $\rho_H/\bar{\rho}$. Obviously, the agreement with experiment is comparable with that in the case of the SMA.

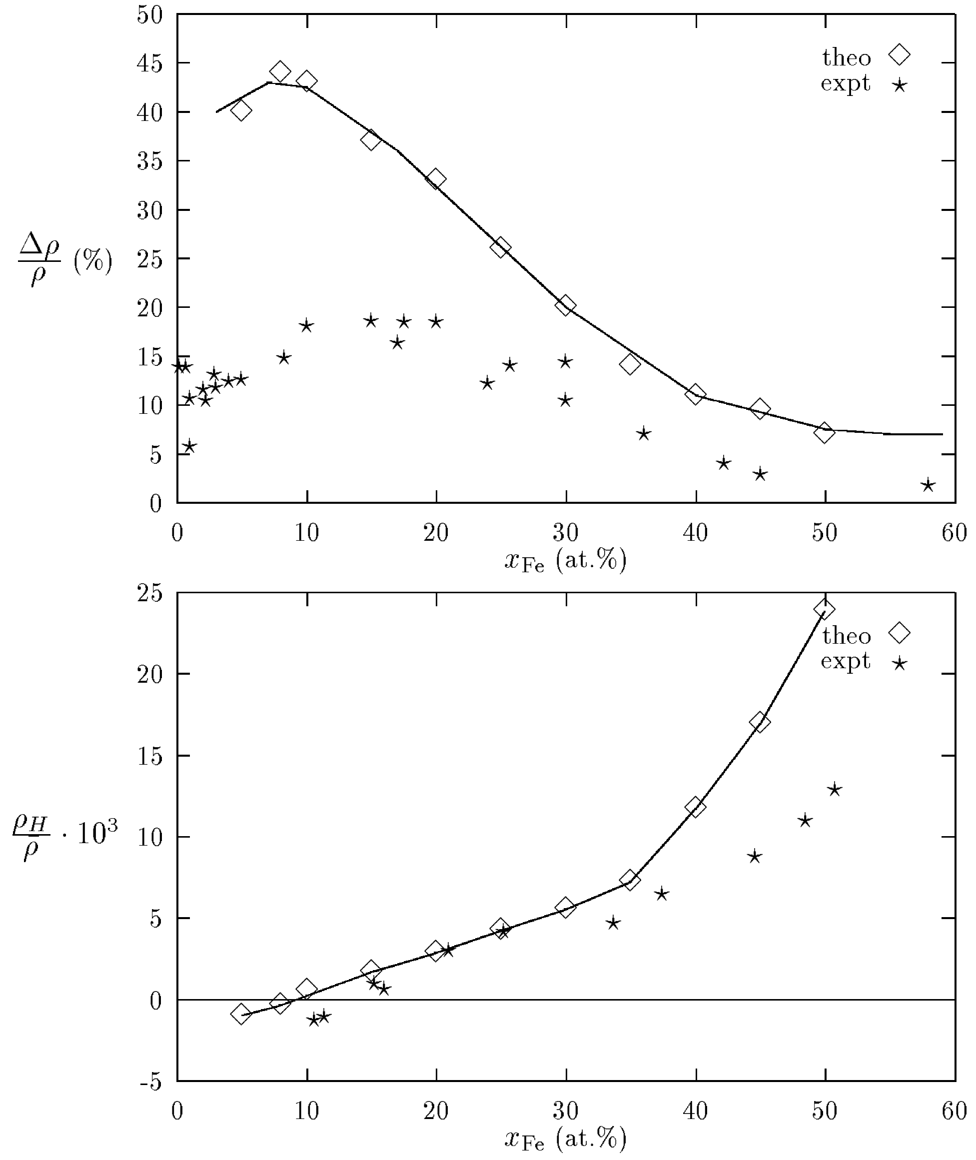

Figure 1: **Top:** Spontanous magneto-resistance anisotropy (SMA) $(\rho_{||} - \rho_{\perp})/\bar{\rho}$ of the disordered alloy system fcc-Fe$_x$Ni$_{1-x}$ for $T = 0K$. **Bottom:** Anomalous Hall resistivity (AHR) of fcc-Fe$_x$Ni$_{1-x}$ expressed by the Hall angle $\rho_H/\bar{\rho}$.

These calculations allowed to study the validity of various assumptions made within previous simple models for the SMA and AHR. For example, it turned out that calculating the SMA based on spin-resolved density of states at the Fermi energy together with a global parameter representing spin-orbit coupling is of rather limited usefullness. A test of the so-called two-current model common to all previous approaches is performed next. Evaluating the relevant matrix elements in the $\boldsymbol{\nabla}$-form (see Eq. (10)) it was found that the additional terms that allow for spin-flip scattering events are by a factor of 100 smaller than the $\boldsymbol{\nabla}$-related part. This means that hybridisation of states with different spin character due to spin-orbit coupling is by far the most important source for the SMA and AHR.

Finally, one should emphasize that the results presented here clearly demonstrate that the *spin only* Hamiltonian in Eq. (1) contains all the relevant physics to allow for a proper description of the SMA and AHR.

6 Magneto-optical Kerr-effect

Any material with a non-diagonal conductivity tensor $\boldsymbol{\sigma}(\omega)$ will in general turn incoming linearly polarised light into elliptically polarized one. If this property of $\boldsymbol{\sigma}(\omega)$ is – at least partly – due to the magnetisation then the effect observed in reflection is called magneto-optical Kerr-effect. The complex Kerr-angle $\phi_K = \theta_K + i\epsilon_K$ combines the Kerr-rotation angle θ_K of the polarisation ellipsis, with respect to the original polarisation vector, and its ellipticity ϵ_K. For a system with at least 3-fold symmetry (i.e. trigonal, hexagonal, tetragonal and cubic) and the magnetisation as well as the incoming beam along the surface normal $\hat{\mathbf{z}}$ (polar geometry) the complex Kerr-angle ϕ_K is given by:

$$\phi_K = \frac{-\sigma_{xy}}{\sigma_{xx}\sqrt{1 + i\left(\frac{4\pi}{\omega}\right)\sigma_{xx}}}\,. \tag{12}$$

In principle the version of the Kubo-Greenwood-equation (8) for finite frequencies could be used in a straightforward way to calculate $\boldsymbol{\sigma}(\omega)$ and from that $\phi_K(\omega)$. Alternatively, one can calculate the absorptive parts of σ_{xx} and σ_{xy} using the expressions:

$$\sigma^{(1)}_{xx} = \frac{\pi e}{2\hbar\omega m V} \sum_{\substack{n\,\mathbf{k}\,\text{occupied} \\ n'\,\mathbf{k}\,\text{unoccupied}}} \left[|<n'\mathbf{k}|\,j_-\,|n\mathbf{k}>|^2 + |<n'\mathbf{k}|\,j_+\,|n\mathbf{k}>|^2 \right] \delta(\omega_{nn'} - \omega) \tag{13}$$

$$\sigma^{(2)}_{xy} = \frac{\pi e}{2\hbar\omega m V} \sum_{\substack{n\,\mathbf{k}\,\text{occupied} \\ n'\,\mathbf{k}\,\text{unoccupied}}} \left[|<n'\mathbf{k}|\,j_-\,|n\mathbf{k}>|^2 - |<n'\mathbf{k}|\,j_+\,|n\mathbf{k}>|^2 \right] \delta(\omega_{nn'} - \omega) \tag{14}$$

and determine the corresponding dispersive parts by a Kramers-Kronig transformation. With $j_\pm = j_x \pm i j_y$ Eqs. (13) and (14) emphasize that $\sigma^{(1)}_{xx}$ and $\sigma^{(2)}_{xy}$ can be viewed respectively as the average and difference of the absorption coefficients for the left and right circularly polarized light.

The expressions in Eqs. (13) and (14) represent only contributions due to $\mathbf{k}$-conserving interband transitions ($n \neq n'$). The intraband transitions are conventionally taken into account in a phenomenological way by the so-called Drude term. Fortunately, this contribution to $\boldsymbol{\sigma}$ can safely be neglected for $\omega \gtrsim 1.5 - 2$ eV.

The form of $\boldsymbol{\sigma}$ given in Eqs. (4) and (5) expresses the fact that changing the orientation of $\mathbf{M}$ from [001] to [110] the true symmetry of the system changes from tetragonal to orthorhombic. From this one can expect a corresponding anisotropy for the Kerr spectra $\theta_K(\omega)$. As can be seen in Fig. 2 this anisotropy is found to be completely neglegible for fcc-Co [7]. This finding is in full agreement with the experimental data of Weller et al. [8] for Co-films with [001]- and [110]-orientation. Obviously, spin-orbit coupling in fcc-Co is responsible for the Kerr-effect

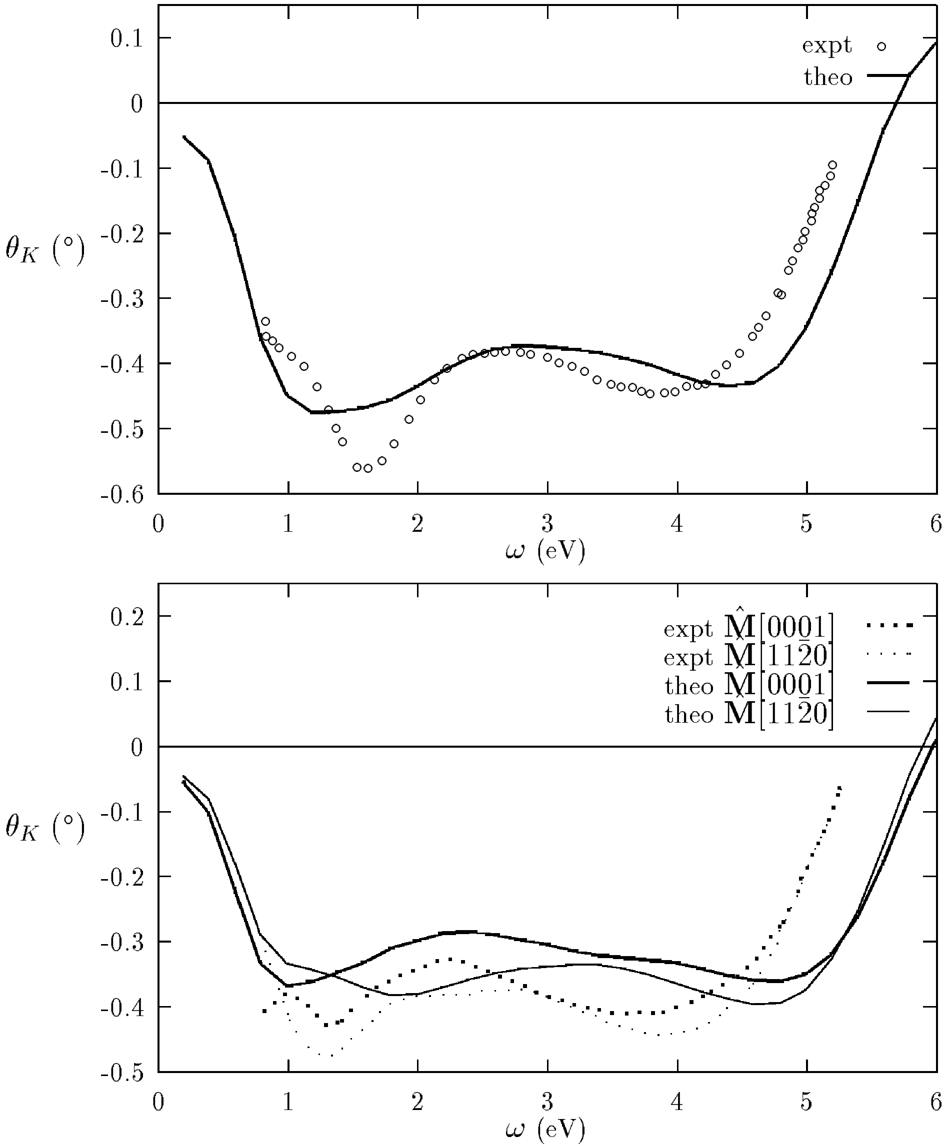

Figure 2: **Top:** Kerr-rotation angle θ_K for fcc-Co with $\hat{\mathbf{M}}[001]$ and $\hat{\mathbf{M}}[110]$. The theoretical spectra for both orientations practically coincide. For the experimental curves only small differences have been found. **Bottom:** Kerr-rotation angle θ_K for hcp-Co with $\hat{\mathbf{M}}[0001]$ and $\hat{\mathbf{M}}[11\bar{2}0]$.

but it is too weak to produce any significant anisotropy for $\theta_K(\omega)$. This situation is similar to the spin-orbit induced field gradient in cubic magnetic solids. This phenomenon, like the Kerr-effect, is a direct manifestation of the reduced symmetry compared to the paramagnetic state. However, even for 5d-elements in an Fe-matrix no significant anisotropy for the field gradient could be detected so far. For hcp-Co the situation completely differs from that for fcc-Co. Here, because of the crystal structure the optical properties are anisotropic even for the paramagnetic state. Thus the anisotropy induced by the magnetic state is superimposed onto that due to the crystal structure. For this reason, in contrast to fcc-Co, there is a clear anisotropy present as can be seen in Fig. 2. Again the experimental data were obtained by

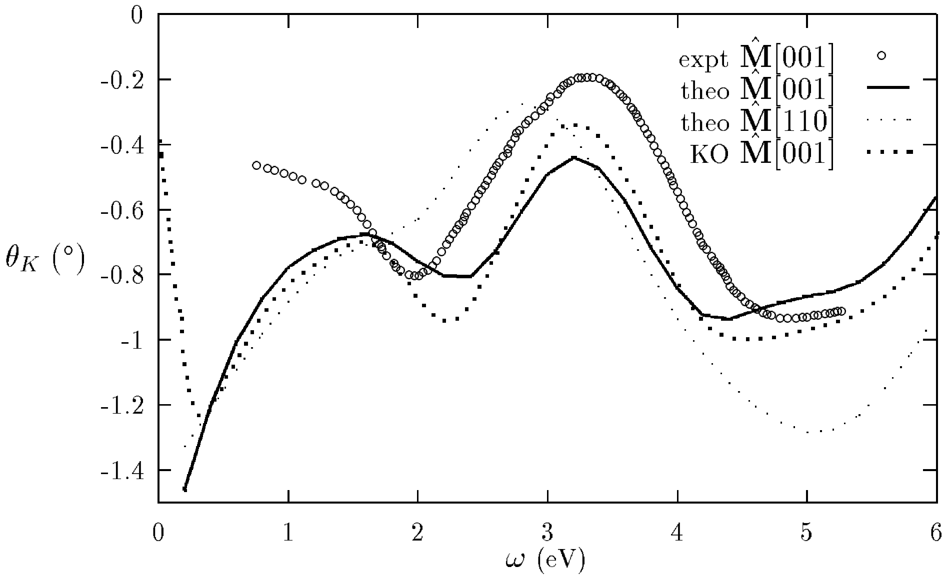

Figure 3: Kerr-rotation angle θ_K for FePt for various orientations. KO stands for Kübler, Oppeneer et al.

Weller et al. for films with [0001]- and [11$\bar{2}$0]-orientation. In line with the anisotropy of θ_K an anisotropy for the total magnetic moment and the hyperfine fields is found (0.004 μ_B and 5.7 kG compared to the experimental values 0.008 μ_B and 8 kG, respectively). In both cases the anisotropy is due to their orbital parts which occur – like θ_K – due to the spin-orbit coupling. However, θ_K gives more detailed (at least partly) energy resolved information on the anisotropy while the orbital moments and hyperfine fields are integral properties of the occupied states.

The hcp-Co could be viewed as a simple layered structure system. For this reason one can expect that the anisotropy of θ_K is more pronounced for a true layered structure, e.g., for the compound FePt in the CuAu-structure. This indeed can be seen from the theoretical spectra in Fig. 3 [9]. Remembering the role of the Drude contribution for $\omega \lesssim 1-2$ eV our results for the [001]-orientation are in fairly good agreement with the experimental results of Weller et al. It seems that so far the preparation of the corresponding films for the [110]-orientation has not been successful. In Fig. 3 we have included the theoretical results of Kübler, Oppeneer et al. [10]. This group is using the scalar-relativistic ASW and accounting for spin-orbit coupling in the variational step, while the results presented so far were obtained using the SPRLMTO-ASA. Because the spectra agree as far as one might expect for two completely different calculations (using presumably slightly different atomic radii, lattice constants and lifetime parameters) one can conclude that: i) for calculating Kerr-spectra and other spin-orbit induced properties it is in general not necessary to use the approach based on the Dirac equation (see Eq. (1)) – even for systems containing heavy elements like Pt, ii) because in the ASW-calculations of Fig. 3 the interstitial region is treated more accurately it is obvious that evaluating the matrix elements of $\mathbf{j}$ in the $\boldsymbol{\nabla}$-form essentially cure the problems with the $\boldsymbol{\alpha}$-form.

Furthermore, using Eq. (10) it was found – as before for $\boldsymbol{\sigma}(\omega = 0)$ of $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ – that spin-flip transitions play only a minor role ($\approx$ 1%). Thus the estimate ($\approx$ 10%) often found in the literature seems to be unrealistic.

Finally, it should be emphasized that statement i) does not mean that the Hamiltonian in Eq. (1) does not have any advantages compared to the variational treatment of spin-orbit coupling. For example treating alloy systems within the CPA would be quite cumbersome using the latter approach. Furthermore future developments in relativistic density functional theory will presumably provide a natural extension of the Hamiltonian in Eq. (1).

7 Magnetic X-ray dichroism

In recent years various experimental groups have demonstrated that the magneto-optical Kerr effect (MOKE) can also be observed in the X-ray regime. This means that although the nature of the initial states completly changes – tightly bound core states versus the itinerant valence band states for the optical regime – the physics remains the same. Much easier than observing the MOKE in the X–ray regime is however the corresponding absorption experiment. For a discussion of that experiment it is obviously sufficient to look at the absorptive parts of the elements of $\boldsymbol{\sigma}$. From the form of $\boldsymbol{\sigma}$ in Eq. (4) one can easily see that different kinds of dichroism i.e. dependencies of the absorption on the polarisation of the radiation may occur. The occurence of σ_{xy} gives rise to the circular dichroism meaning that the absorption coefficients for left and right circularly polarized X–rays, μ_+ and μ_-, respectively, are different. From Eq. (13) and (14) one easily sees that $\mu_\pm \propto \sigma^{(1)}_{xx} \pm \sigma^{(2)}_{xy}$. The difference between σ_{xx} and σ_{zz}, giving rise to the SMA for $\omega = 0$, leads to a linear dichroism, i.e. to different absorption coefficients μ_λ for X–ray linearly polarized parallel to $\hat{\mathbf{M}}$ ($\mu_{||} \propto \sigma^{(1)}_{zz}$) and perpendicular to $\hat{\mathbf{M}}$ ($\mu_\perp \propto \sigma^{(1)}_{xx}$). Eqs. (4) and (5) also demonstrate that one can have different kinds of linear dichroism. The one just described occurs if $\hat{\mathbf{M}}$ is fixed and the polarisation vector is changing. But there is another one for the polarisation fixed and the magnetisation rotated, because for example $\sigma^{(1)}_{zz}(\hat{\mathbf{M}}\ [001])$ may differ from $\sigma^{(1)}_{zz}(\hat{\mathbf{M}}\ [110])$.

A very flexible scheme to calculate the absorption coefficient μ_λ was developed some years ago based on the SPRKKR-method. Alternatively, one can also use the SPRLMTO-method to calculate μ_λ in analogy to Eqs. (13) and (14) from

$$\mu_\lambda \propto \sum_{\substack{i\,\text{occupied} \\ n\,\mathbf{k}\,\text{unoccupied}}} | < n\mathbf{k}|\, j_-\, |i> |^2\, \delta(\omega_{ni} - \omega). \tag{15}$$

As stated above only the nature of the initial state has changed from a Bloch state $|n\mathbf{k}>$ to a core state $|i>$. This has the important consequence that the resulting spectra are not

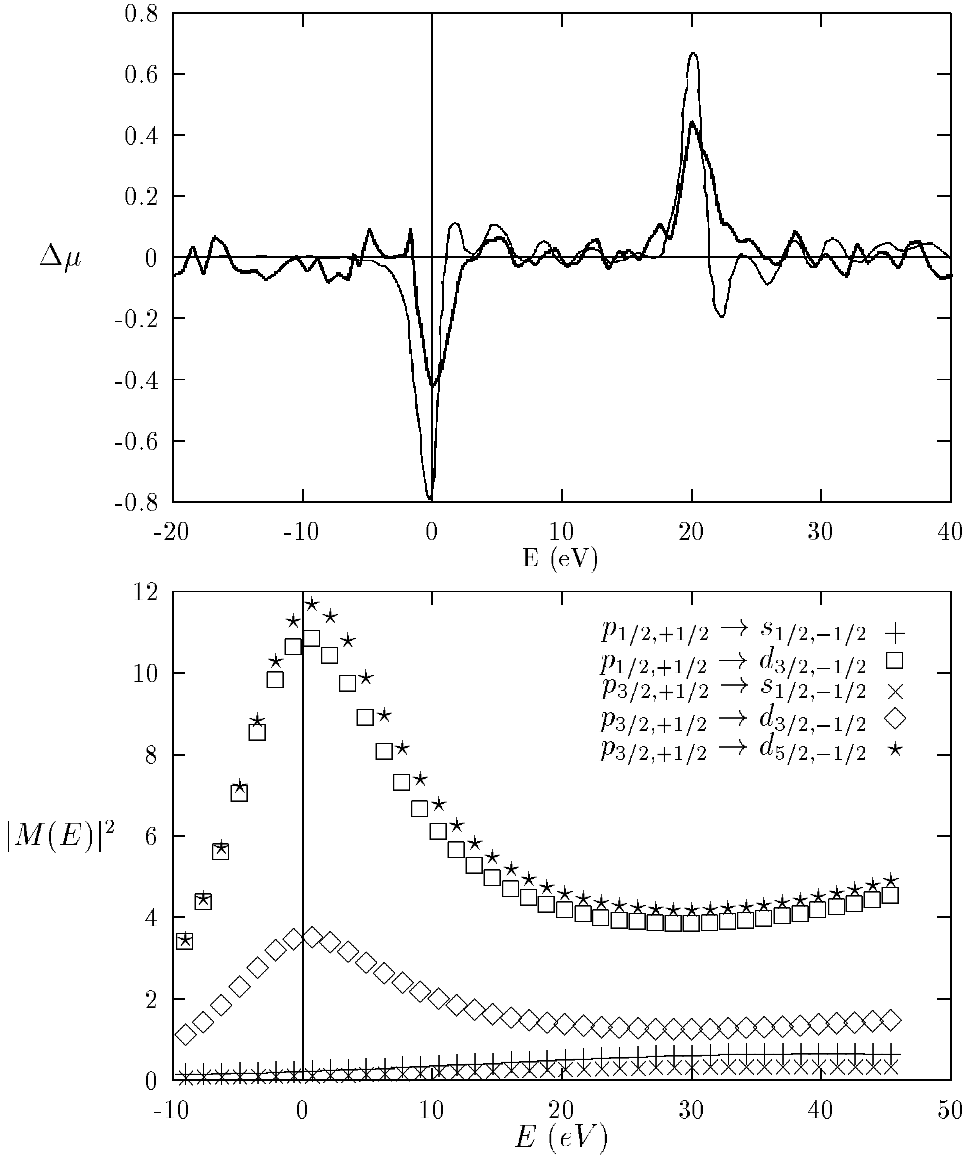

Figure 4: **Top:** Circular dichroism $\Delta\mu = \mu^- - \mu^+$ at the $L_{2,3}$-edge of Cu in the multilayer system Co5/Cu4. Theory: full line, experiment: dashed line. **Bottom:** Matrix elements for the various $2p_{j,\mu} \to 4s(3d)_{j,\mu'}$-transitions with $\mu = +1/2$ and $\mu' = -1/2$ at the $L_{2,3}$-edge of Cu.

anymore linked to the so-called joint density of states but just to the density of unoccupied states. As a result, the interpretation of the resulting spectra is tremendously simplified. Furthermore, again due to the nature of the initial state, the MXD provides a component specific probe of magnetism. This property has been used during the last years for a rapidly increasing number of studies on diluted and concentrated alloys as well as multilayer systems. As an example for such investigations Fig. 4 shows the circular dichroism at the $L_{2,3}$-edge of Cu in the multilayer system Co5/Cu4. Here the difference $\Delta\mu$ of the absorption coefficients for left and right circularly polarized radiation, μ^- and μ^+, resp., has been used as a measure for the dichroism, with the step at the absorption edge normalized to 100. Although the dichroism signal is quite small (of the order of 1 %), it nevertheless reflects the polarisation of the Cu d-band states by the adjacent Co-layers. In most cases $\Delta\mu$ can be viewed as an energy-resolved probe for the spin-polarisation of the final states. From the same sign of $\Delta\mu$ for Cu and Co (not shown here) in Co5/Cu4 one can therefore conclude that the Cu- and Co-moments are aligned in parallel – in accordance with the results of the bandstructure calculation. Using so-called sum rules (see references in [11]), which supply a basis for the above interpretation, a spin magnetic moment of around $0.014\mu_B$ could be deduced from the experimental spectra for Cu. This is in good agreement with the theoretical result ($0.0137\mu_B$). However, one has to keep in mind that one only gets an average value that way. For Co5/Cu4 this means an average for the two inequivalent Cu-layers. In more complex situations as for example Co2/Pt7 one has more inequivalent layers and may encounter corresponding partial spectra with different sign.

The reliability of the sum rules to deduce spin as well as orbital moments from MXD-spectra has recently been investigated in detail [11]. Comparing calculated moments of multilayer systems with moments deduced from corresponding MXD-spectra using the sum rules differences up to 40 % were found. For the orbital moment, for which the application of the sum rules is somewhat simpler, the ratio of the calculated and deduced values was found to be close to 0.67 in all cases.

Although the sum rules applied to experimental spectra gave so far reasonable estimates for the spin and orbital moments in a great variety of systems one should emphasize that these estimates strongly depend on the filtering of the MXD-spectra from the raw data i.e. on the background subtraction. On the other hand one should also emphasize that one of the basic assumptions in deriving the sum rules, namely energy independent radial matrix elements, is rarely fulfilled. Fig. 4 shows corresponding data for the $L_{2,3}$-edge of Cu. As one can see the most important matrix elements vary nearly by 50 % in the energy range $(E - E_F) = 0 - 10eV$. In addition one finds that the $p \to d$-matrix elements are much larger than those of the $p \to s$-transitions. This is, of course, primarily caused by the fact that the relevant $2p-$ and $3d-$radial wavefunctions are nodeless while the $4s-$function has three nodes. As a consequence of this the MXD-spectrum in Fig. 4 is dominated by $p \to d$-transitions although for Cu the $s-$, $p-$ and $d-$densities of states above the Fermi level are of the same order of magnitude.

8 Concluding remarks

The linear response conductivity tensor $\boldsymbol{\sigma}(\omega)$ has been used to demonstrate close relations between various phenomena which at first sight seem to be quite different in nature. Considering the symmetry properties of $\boldsymbol{\sigma}(\omega)$ it becomes obvious that it is spin-orbit coupling together with spin-polarisation that gives rise to the spontanous magnetoresistance anisotropy, the anomalous Hall resistivity, the magneto-optical Kerr-effect, the magnetic X-ray dichroism and so on. Of course dealing with spectroscopies that are influenced by surface properties — as for example the spin- and angle-resolved UPS — the situation may be more complicated and the symmetry considerations may have to be extended accordingly.

The examples presented here demonstrate that used here spin-only Dirac-Hamiltonian provides a firm basis for a theoretical investigation of the various spin-orbit induced phenomena in magnetic solids. However, there are also clear indications coming primarily from MXD-spectroscopy of shortcomings to this approach. These might be linked to the observation that the calculated orbital moments in general turn out to be too small. Obviously further work in that direction needs to be done.

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